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HyperFlow Theory Manual

F. F. Felker

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HyperFlow Theory Manual

Fort Felker
Thermal Fluids Group
New Technologies Engineering Division
Lawrence Livermore National Laboratory

1. Summary

This document presents the underlying theory for an unsteady computational model of the transient aerothermodynamics of a deformable vehicle entering an atmosphere at hypersonic speeds. Many unique features of the problem require unusual computational capabilities. The large accelerations associated with the vehicle's flight dynamics results in the body-fixed reference frame being non-inertial, and the governing equations must be modified to include this effect. The vehicle's structural deformations and ablation requires the inclusion of the effects of a moving solid boundary, with a nonuniform mass flux across that boundary. A computational chemistry capability must be included to treat the thermochemical nonequilibrium of the high-temperature gas dynamics, and the reactions between the ablation products and the dissociated air. The theory required to treat these phenomena are described in this report.

Editor's note: The present document records the computational formulation developed during the first six months of an envisioned three-year LDRD project. At that time a unique opportunity in the private sector led to Fort's resignation from the Laboratory. While admitting the disappointment of having the project terminated prematurely, we also wish to acknowledge that this solid piece of work has created a firm foundation upon which future efforts can build.

2. Nomenclature

The range of physical models required to treat the re-entry vehicle aerothermodynamics problem is quite broad. It was therefore essential to develop a consistent, easy-to-follow notation system for the exposition of the mathematical model. A number of notation conventions are used throughout this document. A vector arrow over a symbol, e.g. \vec{a} , indicates that it is a directional quantity. Specific components of the directional quantity are denoted using subscripts to the right of the symbol, e.g. a_d . The dummy index d , for *direction*, is used to denote specific components of a directional quantity. The lower right subscript can also be used to refer to a specific location in the computational mesh, e.g. $U_{i,j,k}$. Reference to a particular species is made with the right superscript, e.g. ρ^s . A descriptor for a symbol is placed in the left superscript position, e.g. $^{lam}\mu$ for the laminar viscosity. An *effective* quantity, usually including the effects of multiple species or multiple physical processes, is denoted with an overbar, e.g. \bar{R} . A dot over a quantity, e.g. $\dot{\rho}^s$, is used to denote the rate of production (source term) for that quantity within a control volume. Roe-averaged quantities have a carat, e.g. $\hat{\rho}$. Arrays are denoted in boldface, e.g. \mathbf{U} . The Einstein (or indicial) summation convention, where a repeated index denotes summation over all dimensions, is not used in this document: all sums are explicitly defined, nor do commas in indices denote differentiation.

\vec{a}	inertial acceleration vector
$^\alpha \vec{a}$	inertial acceleration vector from angular acceleration
$^{cen} \vec{a}$	inertial acceleration vector from centripetal acceleration
$^{cor} \vec{a}$	inertial acceleration vector from coriolis acceleration
$^{org} \vec{a}$	linear acceleration of origin of noninertial reference frame
a_d	inertial acceleration in d direction
\mathbf{A}	flux Jacobian
$^{con} \mathbf{A}$	convective flux Jacobian
$^\pm \mathbf{A}$	convective flux Jacobian with positive and negative eigenvalues, respectively, used in Steger-Warming flux splitting
$ \hat{\mathbf{A}} $	magnitude of convective flux Jacobian in Roe's method
A^s, B^s, C^s	constants in viscosity model for species s
\mathbf{B}	source Jacobian
c	frozen speed of sound
c^s	species concentration ρ^s / ρ
\bar{c}_p	mass-averaged specific heat at constant pressure
\bar{c}_v	mass-averaged specific heat at constant volume
c_p^s	specific heat at constant pressure for species s
c_v^s	specific heat at constant volume for species s
$^* c_v^s$	effective local specific heat at a flux boundary for species s
$^r c_v^s$	rotational specific heat at constant volume of species s
$^{tr} c_v^s$	translational specific heat at constant volume of species s
$^v c_v^s$	vibrational specific heat at constant volume of species s

D	matrices used in implicit time integration schemes
D^s	diffusion coefficient of species s
\bar{e}	mass-averaged internal energy
e^s	internal energy per unit mass of species s
$^{eq}e^s$	internal energy per unit mass of species s that is in thermodynamic equilibrium
$^ve^s$	vibrational energy per unit mass of species s
E	total energy per unit volume
E	eigenvectors of $\mathbf{S} \frac{\partial^{con}\mathbf{F}}{\partial \mathbf{V}}$
$\hat{\mathbf{E}}$	E matrix computed with Roe-averaged variables
\mathbf{E}^{-1}	inverse of E
$\hat{\mathbf{E}}^{-1}$	\mathbf{E}^{-1} matrix computed with Roe-averaged variables
$^vE^r$	vibrational energy per unit volume of species r
F	flux vector
$^{con}\mathbf{F}$	convective flux vector
$^{con}\hat{\mathbf{F}}$	convective flux vector computed with Roe's flux-splitting method
$^{vis}\mathbf{F}$	viscous flux vector
^{tot}h	total enthalpy
h^s	specific enthalpy of species s
$^fh^s$	heat of formation of species s
fH	total heat of formation per unit volume of all species
k	numerical parameter used in calculation of ψ
^{ref}L	reference length
\vec{m}	momentum vector
m_d	momentum in d direction
m_{\max}	maximum number of iterations in Data-Parallel Line Relation (DPLR) method
\bar{M}	mass-averaged molecular weight
M^s	molecular weight of species s
n	time step number
\vec{n}	unit normal vector
n_d	d^{th} component of \vec{n}
NV	number of vibrational energy modes
NS	number of species
NT	number of turbulence variables
p	pressure
$^{eq}\vec{q}$	equilibrium heat flux vector
^{neq}q	normal component of equilibrium heat flux vector
$^v\vec{q}^r$	vibrational heat flux vector of species r
$^{nv}q^r$	normal component of vibrational heat flux vector of species r
\vec{r}	position vector from origin of noninertial reference frame to fluid particle
r_d	d^{th} component of position vector in noninertial reference frame
R	residual
R	universal gas constant

\bar{R}	mass-averaged gas constant
R^s	species gas constant of species s
sv	inverse of the index list vs . sv provides the vibrational energy number that corresponds to a given species, if present
S	finite volume cell surface, or cell surface area
\mathbf{S}	matrix of partial derivatives of primitive variables with respect to conserved quantities
$\hat{\mathbf{S}}$	\mathbf{S} matrix computed with Roe-averaged variables
\mathbf{S}^{-1}	matrix of partial derivatives of conserved quantities with respect to primitive variables
$\hat{\mathbf{S}}^{-1}$	\mathbf{S}^{-1} matrix computed with Roe-averaged variables
^{lam}S	laminar Schmidt number of fluid mixture
tS	turbulent Schmidt number of fluid mixture
t	time
Δt	time step size
T	temperature
^{ref}T	reference temperature
$^vT^r$	vibrational temperature of species r
$^tu^i$	i^{th} turbulence model variable
\mathbf{U}	vector of conserved quantities
$\mathbf{U}_L, \mathbf{U}_R$	vector of reconstructed conserved quantities on the left and right side, respectively, of a mesh cell surface
\vec{v}	fluid velocity vector
$^{con}\vec{v}$	convective velocity vector
v_d	fluid velocity in d direction
$^D\vec{v}^s$	diffusion velocity of species s
$^{nD}v^s$	normal component of diffusion velocity of species s
ev	effective velocity; normal component of convective velocity
nv	normal velocity; normal component of fluid velocity
^{ref}v	reference velocity
$^S\vec{v}$	surface velocity vector of finite volume cell surface
vs	vibrational species index list that provides the species number that corresponds to a given vibrational energy
V	volume of finite volume cell
\mathbf{V}	vector of primitive variables
\mathbf{W}	source vector for conserved quantities
\vec{x}	spatial coordinate
x_d	d^{th} spatial coordinate
X^s	molar concentration of species s
$\vec{\alpha}$	angular acceleration vector of noninertial reference frame
α_d	d^{th} component of angular acceleration
β	$\bar{\gamma} - 1$

$\delta_{i,j}$	Kronecker delta
$\delta \mathbf{U}$	change in conserved quantities over a time step
ε	small number used to ensure that derivatives of eigenvalues are continuous
ϕ^s	parameter in Wilke mixing model for species s
$\bar{\gamma}$	mass-averaged ratio of specific heats
κ	total conductivity
κ^s	conductivity of species s
$^{lam} \kappa$	laminar component of total conductivity
$^t \kappa$	turbulent component of total conductivity
$^v \kappa^s$	conductivity of vibrational energy
λ	diagonal matrix containing eigenvalues of $\mathbf{S} \frac{\partial^{con} \mathbf{F}}{\partial \mathbf{V}}$
$^{\pm} \lambda$	diagonal matrices containing positive and negative eigenvalues of $\mathbf{S} \frac{\partial^{con} \mathbf{F}}{\partial \mathbf{V}}$, respectively
$^{\pm} \lambda_i$	individual eigenvalues of $^{\pm} \lambda$
$ \hat{\lambda} $	diagonal matrix containing absolute values of eigenvalues of $\mathbf{S} \frac{\partial^{con} \mathbf{F}}{\partial \mathbf{V}}$, computed using Roe-averaged variables
μ	total viscosity
μ^s	viscosity of species s
$^{lam} \mu$	laminar component of total viscosity
$^t \mu$	turbulent component of total viscosity
$^v \theta^s$	characteristic temperature of vibration of species s
ρ	total fluid density
ρ^s	density of species s
$\dot{\rho}^s$	rate of production of species s from chemical reactions
$^{ref} \rho$	reference density
τ	shear stress tensor
$\tau_{i,j}$	i,j component of shear stress tensor
$\vec{\Omega}$	angular acceleration vector of noninertial reference frame
Ω_d	d^{th} component of angular acceleration
ψ	parameter for setting spatial accuracy of reconstruction

3. Introduction

The engineering analysis of the complete aerothermodynamic environment of a re-entry vehicle is a challenging problem. At the hypersonic speeds of planetary re-entry the atmosphere's molecules dissociate in response to the high temperatures generated by the bow shock. The heat flux into the body can be large enough to break down the thermal protection materials, and the resulting products chemically react with the high temperature gas. These reactions cause the geometry of the body to change with time. Structural deformations also change the shape of the body. Finally, the flight dynamics of the vehicle result in large accelerations, and the body-fixed frame of reference is not inertial. An analysis specifically designed to address the aerothermodynamics of maneuvering, deforming, re-entry vehicles has been developed. This document presents the underlying theory for the analysis.

In this initial version of the formulation, some potentially important physical phenomena are neglected. For example, a separate temperature for the electrons is not included, so that the electron temperature is assumed to equal the translation-rotation temperature. These simplifications have been made in order to provide an initial computational capability in as short a time as possible. Follow-on work will be needed to assess the importance of these simplifications, and to develop a more comprehensive theory where needed.

4. Scope of Analysis

The primary assumption made is that due to the relatively simple geometry of re-entry vehicles, a structured mesh attached to the body is an expedient spatial discretization. It is envisioned that eventually the flow region will be coupled to a suitable finite-element based representation of the body. Being attached to the body places the flow mesh in a non-inertial frame and makes it subject to deformations of the boundary coincident with the fluid-solid interface.

5. Thermodynamic Model and Equations of State

Following the work of Grossman and Cinnella (1990), the thermodynamic model allows the internal energy of each species to consist of a part in thermodynamic equilibrium, and a part that is not in equilibrium. The part that is not in equilibrium is regarded here as arising from vibrational energy modes and will be referred to as the vibrational energy. The internal energy per unit mass is then

$$e^s = {}^{eq}e^s + {}^v e^s \quad (5.1)$$

The temperature is associated with the equilibrium internal energy. The equilibrium internal energy is the heat of formation plus the integral of the specific heat at constant volume, with the specific heat regarded as an arbitrary function of temperature.

$${}^{eq}e^s = {}^f h^s + \int_0^T c_v^s(\theta) d\theta \quad (5.2)$$

$$c_v^s = \frac{d^{eq} e^s}{dT} \quad (5.3)$$

Although free electrons can be included as a species, in the present model a separate electron temperature is not included. Also, the electronic excitation energy of bound electrons is not considered, since Grossman and Cinnella (1988) show that the electronic excitation energy is not significant for flows in air.

The gas is a mixture of many species, and it is convenient to define the following average quantities

$$\rho = \sum_{s=1}^{NS} \rho^s \quad (5.4)$$

$$\bar{e} = \sum_{s=1}^{NS} \frac{\rho^s}{\rho} e^s \quad (5.5)$$

$$\bar{c}_v = \sum_{s=1}^{NS} \frac{\rho^s}{\rho} c_v^s \quad (5.6)$$

$$\bar{c}_p = \sum_{s=1}^{NS} \frac{\rho^s}{\rho} c_p^s \quad (5.7)$$

$$\bar{R} = \bar{c}_p - \bar{c}_v = \sum_{s=1}^{NS} \frac{\rho^s}{\rho} \frac{R}{M^s} \quad (5.8)$$

$$\bar{\gamma} = \frac{\bar{c}_p}{\bar{c}_v} = \frac{\bar{R}}{\bar{c}_v} + 1 \quad (5.9)$$

$$^f H = \sum_{s=1}^{NS} \rho^s ^f h^s \quad (5.10)$$

The total energy per unit volume is the sum of the internal energy per unit volume and the fluid kinetic energy

$$E = \rho \bar{e} + \frac{1}{2} \rho \vec{v}^2 \quad (5.11)$$

An implicit equation for the temperature can be obtained by expanding eqn. (5.11) to bring the temperature into evidence

$$E - \frac{1}{2} \rho \vec{v}^2 - \sum_{s=1}^{NV} \rho^s e^s - ^f H - \sum_{s=1}^{NS} \rho^s \int_0^T c_v^s(\theta) d\theta = 0 \quad (5.12)$$

The temperature is found by solving eqn. (5.12). Since the specific heat is in general a nonlinear function of temperature, this equation must be solved iteratively. Once the temperature has been found, the pressure can be computed from

$$p = \rho \bar{R} T \quad (5.13)$$

Also useful is the frozen speed of sound (see Grossman and Cinnella (1990) for derivation)

$$c^2 = \frac{\bar{\gamma} p}{\rho} \quad (5.14)$$

The vibrational energy is related to the vibration temperature by a harmonic oscillator model

$${}^v e^s = \frac{R^s {}^v \theta^s}{e^{{}^v T^s} - 1} \quad (5.15)$$

where ${}^v \theta^s$ is the characteristic temperature of vibration for that species, and R^s is the species gas constant obtained from the universal gas constant and the species molecular weight.

$$R^s = \frac{R}{M^s} \quad (5.16)$$

Equation (5.15) can be solved for the vibration temperature to yield

$${}^v T^s = \frac{{}^v \theta^s}{\ln \left(\frac{R^s {}^v \theta^s}{{}^v e^s} + 1 \right)} \quad (5.17)$$

The total enthalpy is defined by

$${}^{tot} h = \frac{E + p}{\rho} \quad (5.18)$$

6. Shear Stresses, Heat Fluxes, and Diffusion Velocities

Using Stokes' hypothesis for the bulk viscosity, the shear stress is

$$\tau_{i,j} = -\mu \left(\left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right) - \frac{2}{3} \delta_{i,j} \sum_{d=1}^3 \frac{\partial v_d}{\partial x_d} \right) \quad (6.1)$$

The symmetric shear stress tensor is

$$\boldsymbol{\tau} = \begin{bmatrix} \tau_{11} & \tau_{12} & \tau_{13} \\ \tau_{21} & \tau_{22} & \tau_{23} \\ \tau_{31} & \tau_{32} & \tau_{33} \end{bmatrix} \quad (6.2)$$

The viscosity, μ , is the sum of the laminar and turbulent viscosities

$$\mu = {}^{lam}\mu + {}^t\mu \quad (6.3)$$

The heat conduction flux is governed by the Fourier law

$${}^{eq}\vec{q} = -\kappa \nabla T \quad (6.4)$$

Like the viscosity, the conductivity, κ , is the sum of the laminar and turbulent conductivities

$$\kappa = {}^{lam}\kappa + {}^t\kappa \quad (6.5)$$

For the vibrational energy flux

$${}^v\vec{q}^r = -({}^v\kappa^s + {}^t\kappa) \nabla^v T^r \quad (6.6)$$

Curve fits of the following form are used to compute the viscosity of each species

$$\mu^s = e^{C^s} T^{A^s \ln T + B^s} \quad (6.7)$$

The resulting viscosity is in units of g/(cm-s), and must be converted to the MKS units used in the rest of the analysis. The viscosity coefficients can be found in a variety of sources, including Blottner, *et al.* (1971) and Thompson, *et al.* (1990). The coefficients of thermal conductivity are computed using an Eucken relation

$$\kappa^s = \mu^s \left(\frac{5}{2} {}^{tr}c_v^s + {}^r c_v^s + {}^v c_v^s \right) \quad (6.8)$$

The translational, rotational and vibrational specific heats are

$${}^{tr}c_v^s = \frac{3}{2} R^s \quad (6.9)$$

$${}^r c_v^s = R^s \quad (6.10)$$

$${}^v c_v^s = \frac{\partial^n e^s}{\partial {}^v T^s} \quad (6.11)$$

The vibrational conductivity is computed from

$${}^v\kappa^s = \mu^s {}^v c_v^s \quad (6.12)$$

The total laminar viscosity and laminar conductivity are calculated using Wilke's mixing rule

$$\mu^{lam} = \sum_{s=1}^{NS} \frac{X^s \mu^s}{\phi^s} \quad (6.13)$$

$$\kappa^{lam} = \sum_{s=1}^{NS} \frac{X^s \kappa^s}{\phi^s} \quad (6.14)$$

where

$$X^s = \frac{c^s \bar{M}}{M^s} \quad (6.15)$$

$$\bar{M} = \frac{1}{\sum_{s=1}^{NS} \frac{c^s}{M^s}} \quad (6.16)$$

$$\phi^s = \sum_{r=1}^{NS} X^r \frac{\left(1 + \sqrt{\frac{\mu^s}{\mu^r}} \left(\frac{M^r}{M^s} \right)^{\frac{1}{4}} \right)^2}{\sqrt{8 \left(1 + \frac{M^s}{M^r} \right)}} \quad (6.17)$$

The diffusion velocity is defined from

$${}^D \vec{v}^s \rho^s = -\rho D^s \nabla \left(\frac{\rho^s}{\rho} \right) \quad (6.18)$$

The diffusion coefficient is computed by assuming a constant Schmidt number for all species

$$D^s = \frac{\mu^{lam}}{\rho} + \frac{\mu^s}{\rho} \quad (6.19)$$

7. Conserved Quantities

The vector of conserved quantities, \mathbf{U} , consists of mass, turbulence, energy, and momentum quantities. The variables in \mathbf{U} are ordered as follows: the first NS variables are the densities of the species included in the model. The next NT variables are the turbulence model variables, if present. The following NV variables are the vibrational energies. Note that some species may not have vibrational energies (e.g. monatomic species), so NV will usually be less than NS . The next variable is the total energy. The final three variables are the momentums in the three spatial directions. Note that the order of variables used here differs from the usual ordering of mass, momentum, then energy. The present ordering results in simpler expressions for the similarity transformation matrices used in the flux-splitting method, and this ordering was chosen for that reason.

$$\mathbf{U} = \left\{ \begin{array}{c} \rho^1 \\ \vdots \\ \rho^{NS} \\ \vdots \\ {}^t u^1 \\ \vdots \\ {}^t u^{NT} \\ \vdots \\ {}^v E^1 \\ \vdots \\ {}^v E^{NV} \\ \vdots \\ E \\ \vdots \\ m_1 \\ m_2 \\ m_3 \end{array} \right\} \quad (7.1)$$

The vibrational energies per unit volume are

$${}^v E^r = {}^v e^r \rho^{vs(r)} \quad (7.2)$$

The index list $vs(r)$ gives the species number that corresponds to the r^{th} vibrational energy.

The momentum terms are written m_d instead of the usual form of ρv_d to reinforce the idea that momentum is a fundamental conserved quantity, and not the product of density and velocity. Neither density nor velocity is a fundamental independent quantity. Density is the sum of the species densities, and velocity is computed by dividing the momentum by the density.

$$\vec{v} = \frac{\vec{m}}{\rho} \quad (7.3)$$

8. Finite Volume Discretization

A finite volume scheme is used to discretize the computational domain. Finite volume methods have been shown to provide excellent results for hypersonic flows, and they do not suffer from the indexing overhead of general-purpose finite element methods.

8.1 Definition of Control Volume

A hexahedral finite volume cell with indices i, j, k is shown in Fig. 8.1. The cell has six faces: the ^-i face, the ^+i face, the ^-j face, the ^+j face, the ^-k face, and the ^+k face. The ^-i face is defined by the four ^-i corner points; the ^+j face is defined by the four ^+j corner points, etc.

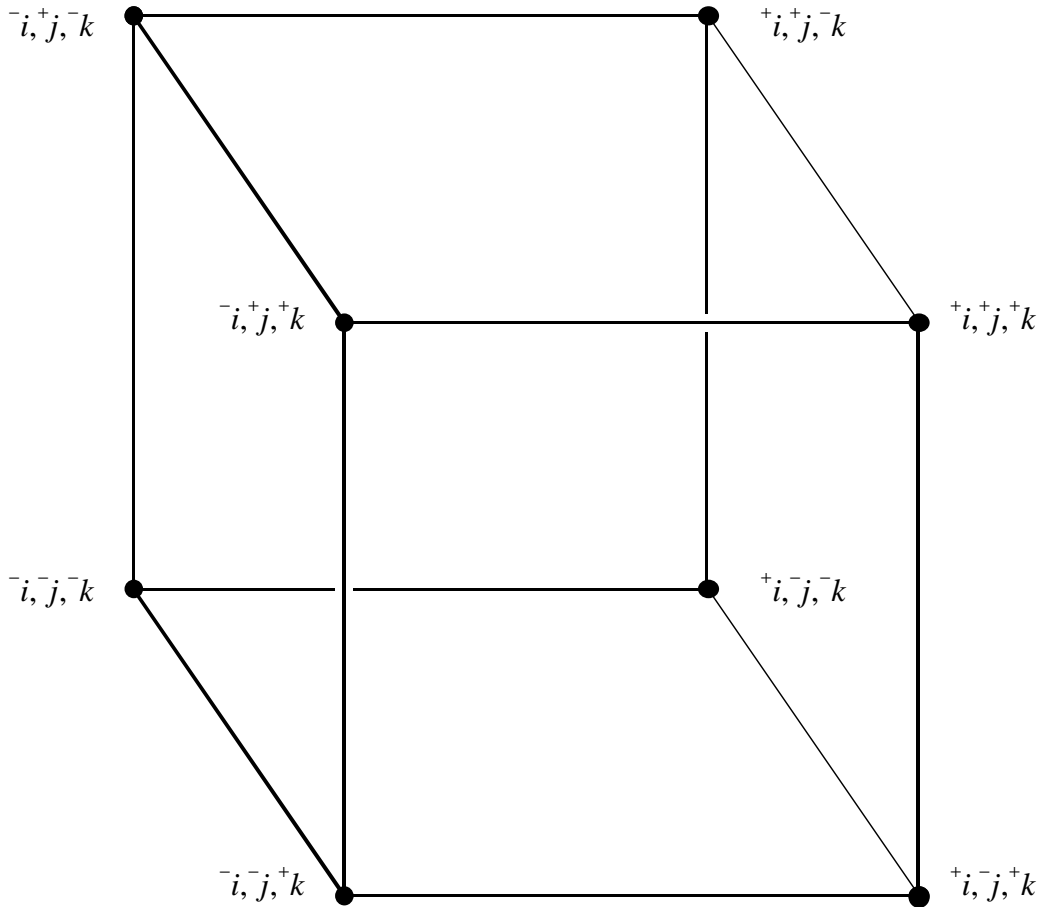


Figure 8.1 Hexahedral finite volume cell with corner point indices.

Although the finite volume cell shown in Fig. 8.1 is a simple cube, we desire the formulation to allow for arbitrary hexahedral shapes. Thus for the present analysis we must also consider that the control volume moves and deforms with time (see Fig. 8.2).

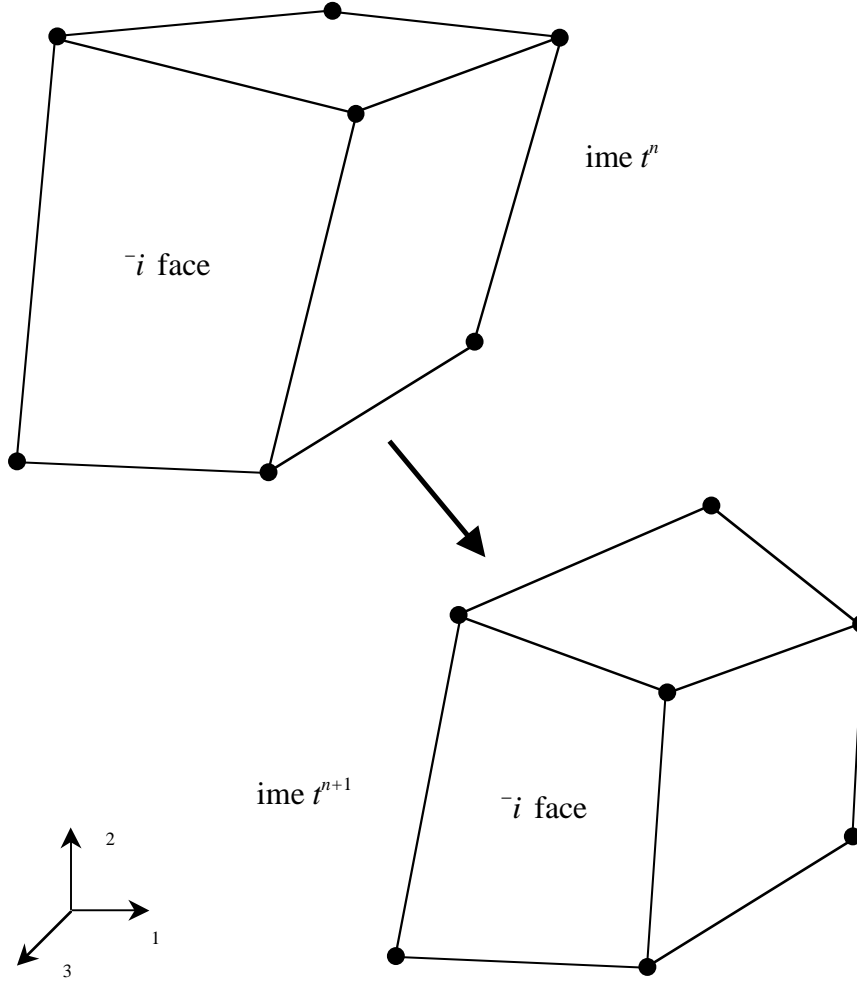


Figure 8.2 Moving, deforming, control volume.

8.2 Computation of Cell Volume, Cell Face Normals, and Cell Face Areas

Formulas for calculating the cell face areas and cell volume are provided in Tannehill, *et al.* (1997). Using the ${}^+i$ face as an example (the other faces are similar), define a face area vector by one half of the cross product of the 2 vectors connecting the diagonally opposite corners (see Fig. 8.1)

$${}^+i\vec{S} = \frac{1}{2} \left({}^+j,{}^+k\vec{r} - {}^-j,{}^-k\vec{r} \right) \times \left({}^-j,{}^+k\vec{r} - {}^+j,{}^-k\vec{r} \right) \quad (8.1)$$

The cell face area is the magnitude of this vector, and the cell face normal vector is the face area vector divided by its magnitude

$${}^+iS = \left| {}^+i\vec{S} \right| \quad (8.2)$$

$${}^+i\vec{n} = \frac{{}^+i\vec{S}}{|{}^+i\vec{S}|} \quad (8.3)$$

The cell volume is one third of the sum of the face area vectors on the ${}^+i$, ${}^+j$, and ${}^+k$ faces, dotted with the diagonal vector from the ${}^-i, {}^-j, {}^-k$ corner to the ${}^+i, {}^+j, {}^+k$ corner

$$V = \frac{1}{3} \left({}^+i\vec{S} + {}^+j\vec{S} + {}^+k\vec{S} \right) \cdot \left({}^+i, {}^+j, {}^+k\vec{r} - {}^-i, {}^-j, {}^-k\vec{r} \right) \quad (8.4)$$

8.3 Indices of Cells and Cell Faces

Within the context of a block-structured hexahedral mesh topology it is straightforward to assign indices to the cells and cell faces. Consider a cell with indices i, j, k . Separate index lists are used to identify the cells, the i faces, the j faces, and the k faces. Within the list of all i faces, the ${}^-i$ face of cell i, j, k has the index i, j, k , and the ${}^+i$ face of that cell has the index $i+1, j, k$. Within the list of all j faces, the ${}^-j$ face of cell i, j, k has the index i, j, k , and the ${}^+j$ face has the index $i, j+1, k$. Within the list of all k faces, the ${}^-k$ face of cell i, j, k has the index i, j, k , and the ${}^+k$ face has the index $i, j, k+1$.

9. Integral Conservation Laws

The conservation laws require that a change in the amount of a conserved quantity inside the control volume must arise from a flux of the conserved quantity across the boundaries of the control volume and/or production of the conserved quantity inside the control volume.

9.1 Conservation of Mass

A mathematical statement of the conservation of species mass is

$$\begin{aligned} \iiint_{V(t^{n+1})} \rho^s(\vec{x}, t^{n+1}) dV - \iiint_{V(t^n)} \rho^s(\vec{x}, t^n) dV &= \int_{t^n}^{t^{n+1}} \left(\iint_{S(t)} \rho^s(\vec{x}, t) {}^S\vec{v}(\vec{x}, t) \cdot \vec{n}(\vec{x}, t) dS \right) dt \\ &+ \int_{t^n}^{t^{n+1}} \left(\iint_{S(t)} \rho^s(\vec{x}, t) (-\vec{v}(\vec{x}, t)) \cdot \vec{n}(\vec{x}, t) dS \right) dt \\ &+ \int_{t^n}^{t^{n+1}} \left(\iint_{S(t)} \rho^s(\vec{x}, t) (-{}^D\vec{v}^s(\vec{x}, t)) \cdot \vec{n}(\vec{x}, t) dS \right) dt \\ &+ \int_{t^n}^{t^{n+1}} \left(\iiint_{V(t)} \dot{\rho}^s(\vec{x}, t) dV \right) dt \end{aligned} \quad (9.1)$$

Term-by-term, this equation states that the total mass in the control volume at time $n+1$, minus the total mass in the control volume at time n , is equal to the mass entering the control volume because of its surface motion during the time interval, plus the mass entering the control volume

by crossing its surface with the fluid flow during the time interval, plus the mass entering the control volume by crossing its surface because of the species diffusion velocity during the time interval, plus the amount of mass produced inside the control volume during the time interval. Recall that the mass production term arises from chemical reactions between the various species present in the flow.

Define the values of the conserved quantities in a cell as their average values over the volume of the cell, and similarly define the source terms in a cell as their average values over the volume of the cell

$$\rho^s(t) \equiv \frac{1}{V(t)} \iiint_{V(t)} \rho^s(\vec{x}, t) dV \quad (9.2)$$

$$\dot{\rho}^s(t) \equiv \frac{1}{V(t)} \iiint_{V(t)} \dot{\rho}^s(\vec{x}, t) dV \quad (9.3)$$

Also, define an effective convective velocity as the difference between the local fluid velocity and the cell surface velocity

$$^{con}\vec{v}(\vec{x}, t) = \vec{v}(\vec{x}, t) - \vec{S}(\vec{x}, t) \quad (9.4)$$

Note that the diffusion velocity is not included in the effective convective velocity. The diffusion velocity arises because of viscous processes, and it is not included in the flux-splitting methodology used for the convective terms. With these definitions eqn. (9.1) can be simplified to

$$\begin{aligned} \rho^s(t^{n+1})V(t^{n+1}) - \rho^s(t^n)V(t^n) = & - \int_{t^n}^{t^{n+1}} \left(\iint_{S(t)} \rho^s(\vec{x}, t) ^{con}\vec{v}(\vec{x}, t) \cdot \vec{n}(\vec{x}, t) dS \right) dt \\ & - \int_{t^n}^{t^{n+1}} \left(\iint_{S(t)} \rho^s(\vec{x}, t) ^D\vec{v}(\vec{x}, t) \cdot \vec{n}(\vec{x}, t) dS \right) dt \\ & + \int_{t^n}^{t^{n+1}} \dot{\rho}^s(t)V(t) dt \end{aligned} \quad (9.5)$$

The area integral on the right hand side of this equation can be replaced by a sum over the six faces of the hexahedral control volume. The values of the variables inside the surface integrals are defined to be their average values over the faces. For example, for the $^{-i}$ face,

$$^{-i}(\rho^s ^{con}\vec{v} \cdot \vec{n}) \equiv \frac{1}{S(^{-i})} \iint_{S(^{-i})} \rho^s(^{-i}) ^{con}\vec{v}(^{-i}) \cdot \vec{n}(^{-i}) dS \quad (9.6)$$

and similarly for the other quantities and the other faces. Then eqn. (9.5) can be rewritten as

$$\begin{aligned}
\rho^s(t^{n+1})V(t^{n+1}) - \rho^s(t^n)V(t^n) = & - \int_{t^n}^{t^{n+1}} \left(\begin{aligned} & \bar{\rho}^s \left(\rho^{s\text{con}} \vec{v} \cdot \vec{n} S \right) + {}^+ \rho^s \left(\rho^{s\text{con}} \vec{v} \cdot \vec{n} S \right) \\ & + \bar{\rho}^s \left(\rho^{s\text{con}} \vec{v} \cdot \vec{n} S \right) + {}^+ \rho^s \left(\rho^{s\text{con}} \vec{v} \cdot \vec{n} S \right) \\ & + \bar{\rho}^s \left(\rho^{s\text{con}} \vec{v} \cdot \vec{n} S \right) + {}^+ \rho^s \left(\rho^{s\text{con}} \vec{v} \cdot \vec{n} S \right) \end{aligned} \right) dt \\
& - \int_{t^n}^{t^{n+1}} \left(\begin{aligned} & \bar{\rho}^s \left(\rho^{sD} \vec{v}^s \cdot \vec{n} S \right) + {}^+ \rho^s \left(\rho^{sD} \vec{v}^s \cdot \vec{n} S \right) \\ & + \bar{\rho}^s \left(\rho^{sD} \vec{v}^s \cdot \vec{n} S \right) + {}^+ \rho^s \left(\rho^{sD} \vec{v}^s \cdot \vec{n} S \right) \\ & + \bar{\rho}^s \left(\rho^{sD} \vec{v}^s \cdot \vec{n} S \right) + {}^+ \rho^s \left(\rho^{sD} \vec{v}^s \cdot \vec{n} S \right) \end{aligned} \right) dt \\
& + \int_{t^n}^{t^{n+1}} \dot{\rho}^s V dt
\end{aligned} \tag{9.7}$$

Note that all terms inside the time integrals in eqn. (9.7) are regarded as functions of time. Several approximations to these time integrals are possible, and the various possibilities will be discussed in Section 21. Also note that in eqn. (9.7) the terms on the right hand side are organized into 3 groups: convective terms, viscous terms, and source terms. Similar groupings will be established for all the integral governing equations, as this allows appropriate numerical treatment of each of these physical processes.

9.2 Conservation of Turbulence Quantities

The turbulence model may include quantities that are conserved and convect with the flow, e.g. turbulent kinetic energy. Let ${}^t u$ represent such a turbulence quantity. Then the integral conservation law can be expressed as

$$\begin{aligned}
\iiint_{V(t^{n+1})} {}^t u(\vec{x}, t^{n+1}) dV - \iiint_{V(t^n)} {}^t u(\vec{x}, t^n) dV = & \int_{t^n}^{t^{n+1}} \left(\iint_{S(t)} {}^t u(\vec{x}, t) {}^s \vec{v}(\vec{x}, t) \cdot \vec{n}(\vec{x}, t) dS \right) dt \\
& + \int_{t^n}^{t^{n+1}} \left(\iint_{S(t)} {}^t u(\vec{x}, t) (-\vec{v}(\vec{x}, t)) \cdot \vec{n}(\vec{x}, t) dS \right) dt \\
& + \int_{t^n}^{t^{n+1}} \left(\iiint_{V(t)} {}^t \dot{u}(\vec{x}, t) dV \right) dt
\end{aligned} \tag{9.8}$$

Term-by-term, this equation states that the turbulence quantity in the control volume at time $n+1$, minus the turbulence quantity in the control volume at time n , is equal to the amount entering the control volume because of its surface motion during the time interval, plus the amount entering the control volume by crossing its surface with the fluid flow during the time interval, plus the amount of the turbulence quantity produced inside the control volume during the time interval.

By applying similar definitions to eqn. (9.8) as were applied to the conservation of mass equation, the above equation can be rewritten as

$$\begin{aligned}
{}^t u(t^{n+1})V(t^{n+1}) - {}^t u(t^n)V(t^n) = & - \int_{t^n}^{t^{n+1}} \left(\begin{aligned} & {}^{-i}({}^t u^{con} \vec{v} \cdot \vec{n} S) + {}^{+i}({}^t u^{con} \vec{v} \cdot \vec{n} S) \\ & + {}^{-j}({}^t u^{con} \vec{v} \cdot \vec{n} S) + {}^{+j}({}^t u^{con} \vec{v} \cdot \vec{n} S) \\ & + {}^{-k}({}^t u^{con} \vec{v} \cdot \vec{n} S) + {}^{+k}({}^t u^{con} \vec{v} \cdot \vec{n} S) \end{aligned} \right) dt \\
& + \int_{t^n}^{t^{n+1}} {}^t \dot{u} V dt
\end{aligned} \tag{9.9}$$

As before, all terms in the above equation that are inside the time integrals are regarded as functions of time. Note that there is no viscous term for this governing equation.

9.3 Conservation of Vibrational Energy

The conservation (balance) of vibrational energy must include the vibrational energy flux across the boundary of the control volume that arises from gradients in the vibrational temperature. Let ${}^v E^r$ be the nonequilibrium energy of species r . Then the conservation of vibrational energy can be defined by

$$\begin{aligned}
\iiint_{V(t^{n+1})} {}^v E^r(\vec{x}, t^{n+1}) dV - \iiint_{V(t^n)} {}^v E^r(\vec{x}, t^n) dV = & \int_{t^n}^{t^{n+1}} \left(\iint_{S(t)} {}^v E^r(\vec{x}, t) {}^S \vec{v}(\vec{x}, t) \cdot \vec{n}(\vec{x}, t) dS \right) dt \\
& + \int_{t^n}^{t^{n+1}} \left(\iint_{S(t)} {}^v E^r(\vec{x}, t) (-\vec{v}(\vec{x}, t)) \cdot \vec{n}(\vec{x}, t) dS \right) dt \\
& + \int_{t^n}^{t^{n+1}} \left(\iint_{S(t)} {}^v E^r(\vec{x}, t) (-{}^D \vec{v}^{vs(r)}(\vec{x}, t)) \cdot \vec{n}(\vec{x}, t) dS \right) dt \\
& + \int_{t^n}^{t^{n+1}} \left(\iint_{S(t)} (-{}^v \vec{q}^r(\vec{x}, t)) \cdot \vec{n}(\vec{x}, t) dS \right) dt \\
& + \int_{t^n}^{t^{n+1}} \left(\iiint_{V(t)} {}^v \dot{E}^r(\vec{x}, t) dV \right) dt
\end{aligned} \tag{9.10}$$

Term-by-term, this equation states that the vibrational energy in the control volume at time $n+1$, minus the vibrational energy in the control volume at time n , is equal to the vibrational energy entering the control volume because of its surface motion during the time interval, plus the vibrational energy entering the control volume by crossing its surface with the fluid flow during the time interval, plus the vibrational energy entering the control volume by crossing its surface because of the species diffusion velocity during the time interval, plus the vibrational energy entering the control volume because of the gradient in vibrational temperature during the time interval, plus the amount of vibrational energy produced inside the control volume during the time interval. The exchange of vibrational energy with translational energy will be discussed further in Section 12.

By defining cell- and face-averaged quantities in the usual manner, this equation can be rewritten as

$$\begin{aligned}
{}^v E^r(t^{n+1})V(t^{n+1}) - {}^v E^r(t^n)V(t^n) = & - \int_{t^n}^{t^{n+1}} \left(\begin{aligned} & {}^{-i}({}^v E^{r\,con} \vec{v} \cdot \vec{n} S) + {}^{+i}({}^v E^{r\,con} \vec{v} \cdot \vec{n} S) \\ & + {}^{-j}({}^v E^{r\,con} \vec{v} \cdot \vec{n} S) + {}^{+j}({}^v E^{r\,con} \vec{v} \cdot \vec{n} S) \\ & + {}^{-k}({}^v E^{r\,con} \vec{v} \cdot \vec{n} S) + {}^{+k}({}^v E^{r\,con} \vec{v} \cdot \vec{n} S) \end{aligned} \right) dt \\
& - \int_{t^n}^{t^{n+1}} \left(\begin{aligned} & {}^{-i}(({}^v E^{rD} \vec{v}^{vs(r)} + {}^v \vec{q}^r) \cdot \vec{n} S) + {}^{+i}(({}^v E^{rD} \vec{v}^{vs(r)} + {}^v \vec{q}^r) \cdot \vec{n} S) \\ & + {}^{-j}(({}^v E^{rD} \vec{v}^{vs(r)} + {}^v \vec{q}^r) \cdot \vec{n} S) + {}^{+j}(({}^v E^{rD} \vec{v}^{vs(r)} + {}^v \vec{q}^r) \cdot \vec{n} S) \\ & + {}^{-k}(({}^v E^{rD} \vec{v}^{vs(r)} + {}^v \vec{q}^r) \cdot \vec{n} S) + {}^{+k}(({}^v E^{rD} \vec{v}^{vs(r)} + {}^v \vec{q}^r) \cdot \vec{n} S) \end{aligned} \right) dt \\
& + \int_{t^n}^{t^{n+1}} {}^v \dot{E}^r V dt
\end{aligned} \tag{9.11}$$

9.4 Conservation of Total Energy

The equation that expresses the conservation of total energy includes an additional term to account for the work done on the fluid by the pressure. Also, no mechanism is considered here that produces energy, so there is no source term in the total energy equation.

$$\begin{aligned}
\iiint_{V(t^{n+1})} E(\vec{x}, t^{n+1}) dV - \iiint_{V(t^n)} E(\vec{x}, t^n) dV = & \int_{t^n}^{t^{n+1}} \left(\iint_{S(t)} E(\vec{x}, t) {}^s \vec{v}(\vec{x}, t) \cdot \vec{n}(\vec{x}, t) dS \right) dt \\
& + \int_{t^n}^{t^{n+1}} \left(\iint_{S(t)} E(\vec{x}, t) (-\vec{v}(\vec{x}, t)) \cdot \vec{n}(\vec{x}, t) dS \right) dt \\
& + \int_{t^n}^{t^{n+1}} \left(\iint_{S(t)} p(\vec{x}, t) (-\vec{v}(\vec{x}, t)) \cdot \vec{n}(\vec{x}, t) dS \right) dt \\
& + \int_{t^n}^{t^{n+1}} \left(\iint_{S(t)} \sum_{s=1}^{NS} \rho^s(\vec{x}, t) h^s(\vec{x}, t) (-{}^D \vec{v}^s(\vec{x}, t)) \cdot \vec{n}(\vec{x}, t) dS \right) dt \\
& + \int_{t^n}^{t^{n+1}} \left(\iint_{S(t)} \sum_{r=1}^{NV} (-{}^v \vec{q}^r(\vec{x}, t)) \cdot \vec{n}(\vec{x}, t) dS \right) dt \\
& + \int_{t^n}^{t^{n+1}} \left(\iint_{S(t)} (-{}^{eq} \vec{q}(\vec{x}, t)) \cdot \vec{n}(\vec{x}, t) dS \right) dt \\
& + \int_{t^n}^{t^{n+1}} \left(\iint_{S(t)} (-\boldsymbol{\tau}(\vec{x}, t) \vec{v}(\vec{x}, t)) \cdot \vec{n}(\vec{x}, t) dS \right) dt
\end{aligned} \tag{9.12}$$

Term-by-term, this equation states that the energy in the control volume at time $n+1$, minus the energy in the control volume at time n , is equal to the energy entering the control volume because of surface motion during the time interval, plus the energy entering the control volume by crossing its surface with the fluid flow during the time interval, plus the work done on the control volume from the product of pressure and fluid velocity during the time interval, plus the species enthalpy entering the control volume by crossing its surface with the species diffusion velocity during the time interval, plus the energy entering the control volume because of the gradient in vibrational temperature during the time interval, plus the energy entering the control volume because of the gradient in equilibrium temperature during the time interval, plus the work done on the control volume from the product of the shear stress tensor and the fluid velocity during the time interval.

Application of the usual volume-averaging procedures leads to

$$\begin{aligned}
 E(t^{n+1})V(t^{n+1}) - E(t^n)V(t^n) = & - \int_{t^n}^{t^{n+1}} \left(\begin{aligned} & {}^{-i} \left((E^{con}\vec{v} + p\vec{v}) \cdot \vec{n}S \right) + {}^{+i} \left((E^{con}\vec{v} + p\vec{v}) \cdot \vec{n}S \right) \\ & {}^{-j} \left((E^{con}\vec{v} + p\vec{v}) \cdot \vec{n}S \right) + {}^{+j} \left((E^{con}\vec{v} + p\vec{v}) \cdot \vec{n}S \right) \\ & {}^{-k} \left((E^{con}\vec{v} + p\vec{v}) \cdot \vec{n}S \right) + {}^{+k} \left((E^{con}\vec{v} + p\vec{v}) \cdot \vec{n}S \right) \end{aligned} \right) dt \\
 & - \int_{t^n}^{t^{n+1}} \left(\begin{aligned} & {}^{-i} \left(\left(\sum_{s=1}^{NS} \rho^s h^s {}^s D \vec{v}^s + \sum_{r=1}^{NV} {}^v \vec{q}^r + {}^{eq} \vec{q} + \vec{\tau} \right) \cdot \vec{n}S \right) + {}^{+i} \left(\left(\sum_{s=1}^{NS} \rho^s h^s {}^s D \vec{v}^s + \sum_{r=1}^{NV} {}^v \vec{q}^r + {}^{eq} \vec{q} + \vec{\tau} \right) \cdot \vec{n}S \right) \\ & {}^{-j} \left(\left(\sum_{s=1}^{NS} \rho^s h^s {}^s D \vec{v}^s + \sum_{r=1}^{NV} {}^v \vec{q}^r + {}^{eq} \vec{q} + \vec{\tau} \right) \cdot \vec{n}S \right) + {}^{+j} \left(\left(\sum_{s=1}^{NS} \rho^s h^s {}^s D \vec{v}^s + \sum_{r=1}^{NV} {}^v \vec{q}^r + {}^{eq} \vec{q} + \vec{\tau} \right) \cdot \vec{n}S \right) \\ & {}^{-k} \left(\left(\sum_{s=1}^{NS} \rho^s h^s {}^s D \vec{v}^s + \sum_{r=1}^{NV} {}^v \vec{q}^r + {}^{eq} \vec{q} + \vec{\tau} \right) \cdot \vec{n}S \right) + {}^{+k} \left(\left(\sum_{s=1}^{NS} \rho^s h^s {}^s D \vec{v}^s + \sum_{r=1}^{NV} {}^v \vec{q}^r + {}^{eq} \vec{q} + \vec{\tau} \right) \cdot \vec{n}S \right) \end{aligned} \right) dt \quad (9.13)
 \end{aligned}$$

9.5 Conservation of Momentum

For the conservation of momentum equation, the change in momentum from the pressure must be included, as well as the source term that arises from the noninertial reference frame. See Section 13 for the details of the noninertial reference frame source term.

$$\begin{aligned}
\iiint_{V(t^{n+1})} m_d(\vec{x}, t^{n+1}) dV - \iiint_{V(t^n)} m_d(\vec{x}, t^n) dV &= \int_{t^n}^{t^{n+1}} \left(\iint_{S(t)} m_d(\vec{x}, t)^S \vec{v}(\vec{x}, t) \cdot \vec{n}(\vec{x}, t) dS \right) dt \\
&+ \int_{t^n}^{t^{n+1}} \left(\iint_{S(t)} m_d(\vec{x}, t) (-\vec{v}(\vec{x}, t)) \cdot \vec{n}(\vec{x}, t) dS \right) dt \\
&+ \int_{t^n}^{t^{n+1}} \left(\iint_{S(t)} -p(\vec{x}, t) n_d(\vec{x}, t) dS \right) dt \\
&+ \int_{t^n}^{t^{n+1}} \left(\iint_{S(t)} \boldsymbol{\tau}_d(\vec{x}, t) \cdot \vec{n}(\vec{x}, t) dS \right) dt \\
&+ \int_{t^n}^{t^{n+1}} \left(\iiint_{V(t)} -\rho(\vec{x}, t) a_d(\vec{x}, t) dV \right) dt
\end{aligned} \tag{9.14}$$

where $\boldsymbol{\tau}_d$ is the d^{th} row of the shear stress tensor. Term-by-term, this equation, which applies to the d^{th} component of the momentum, states that the momentum in the control volume at time $n+1$, minus the momentum in the control volume at time n , is equal to the momentum entering the control volume because of its surface motion during the time interval, plus the momentum entering the control volume by crossing its surface with the fluid flow during the time interval, plus the change in momentum that arises from the pressure force on the surface of the control volume over the time interval, plus the change in momentum that arises from the viscous shear stress on the surface of the control volume over the time interval, plus the apparent change in momentum that arises from the noninertial motion of the reference frame during the time interval.

Applying volume and surface integrals in the usual manner leads to

$$\begin{aligned}
m_d(t^{n+1})V(t^{n+1}) - m_d(t^n)V(t^n) &= - \int_{t^n}^{t^{n+1}} \left(\begin{aligned} &^{-i} \left((m_d^{\text{con}} \vec{v} \cdot \vec{n} + p n_d) S \right) + ^{+i} \left((m_d^{\text{con}} \vec{v} \cdot \vec{n} + p n_d) S \right) \\ &+ ^{-j} \left((m_d^{\text{con}} \vec{v} \cdot \vec{n} + p n_d) S \right) + ^{+j} \left((m_d^{\text{con}} \vec{v} \cdot \vec{n} + p n_d) S \right) \\ &+ ^{-k} \left((m_d^{\text{con}} \vec{v} \cdot \vec{n} + p n_d) S \right) + ^{+k} \left((m_d^{\text{con}} \vec{v} \cdot \vec{n} + p n_d) S \right) \end{aligned} \right) dt \\
&- \int_{t^n}^{t^{n+1}} \left(\begin{aligned} &^{-i} (-\boldsymbol{\tau}_d \cdot \vec{n} S) + ^{+i} (-\boldsymbol{\tau}_d \cdot \vec{n} S) \\ &+ ^{-j} (-\boldsymbol{\tau}_d \cdot \vec{n} S) + ^{+j} (-\boldsymbol{\tau}_d \cdot \vec{n} S) \\ &+ ^{-k} (-\boldsymbol{\tau}_d \cdot \vec{n} S) + ^{+k} (-\boldsymbol{\tau}_d \cdot \vec{n} S) \end{aligned} \right) dt \\
&+ \int_{t^n}^{t^{n+1}} -\rho a_d V dt
\end{aligned} \tag{9.15}$$

9.6 Convective and Viscous Flux Vectors, and Source Vector

The convective terms in eqns. (9.7), (9.9), (9.11), (9.13), and (9.15) can be collected together to form a single convective flux vector in a manner similar to the organization of the conserved quantities into a single vector in eqn. (7.1). The resulting convective flux vector, for any of the six faces of the hexahedral, is

$${}^{con}\mathbf{F} = S \left\{ \begin{array}{c} \rho^{1e} v \\ \vdots \\ \rho^{NSe} v \\ \hline {}^t u^{1e} v \\ \vdots \\ {}^t u^{NTe} v \\ \hline {}^v E^{1e} v \\ \vdots \\ {}^v E^{NVe} v \\ \hline E^e v + p^n v \\ \hline m_1^e v + p n_1 \\ m_2^e v + p n_2 \\ m_3^e v + p n_3 \end{array} \right\} \quad (9.16)$$

with the effective velocity and the normal velocity defined by

$${}^e v = {}^{con} \vec{v} \cdot \vec{n} \quad (9.17)$$

$${}^n v = \vec{v} \cdot \vec{n} \quad (9.18)$$

Collecting the viscous fluxes into a single vector, we obtain

$${}^{vis}\mathbf{F} = S \left\{ \begin{array}{c} \rho^{1nD} v^s \\ \vdots \\ \rho^{NSnD} v^s \\ \hline 0 \\ \vdots \\ 0 \\ \hline {}^v E^{1nD} v^{vs(1)} + {}^{nv} q^1 \\ \vdots \\ {}^v E^{NVnD} v^{vs(NV)} + {}^{nv} q^{NV} \\ \hline \sum_{s=1}^{NS} \rho^s h^{snD} v^s + \sum_{r=1}^{NV} {}^{nv} q^r + {}^{neq} q + {}^n(\boldsymbol{\tau}\vec{v}) \\ \hline -(\tau_{11}n_1 + \tau_{12}n_2 + \tau_{13}n_3) \\ -(\tau_{21}n_1 + \tau_{22}n_2 + \tau_{23}n_3) \\ -(\tau_{31}n_1 + \tau_{32}n_2 + \tau_{33}n_3) \end{array} \right\} \quad (9.19)$$

where the normal components of the diffusion velocity and the heat fluxes are

$${}^{nD} v^s = {}^D \vec{v}^s \cdot \vec{n} \quad (9.20)$$

$${}^{nv} q^r = {}^v \vec{q}^r \cdot \vec{n} \quad (9.21)$$

$${}^{neq} q = {}^{eq} \vec{q} \cdot \vec{n} \quad (9.22)$$

and the normal component of the shear stress work is

$${}^n(\boldsymbol{\tau}\vec{v}) = (\boldsymbol{\tau}\vec{v}) \cdot \vec{n} \quad (9.23)$$

The source terms can also be collected into a single vector

$$\mathbf{W} = V \left\{ \begin{array}{c} \dot{\rho}^1 \\ \vdots \\ \dot{\rho}^{NS} \\ \dots \\ {}^t\dot{u}^1 \\ \vdots \\ {}^t\dot{u}^{NT} \\ \dots \\ {}^v\dot{E}^1 \\ \vdots \\ {}^v\dot{E}^{NV} \\ \dots \\ 0 \\ \dots \\ -\rho a_1 \\ -\rho a_2 \\ -\rho a_3 \end{array} \right\} \quad (9.24)$$

9.7 Vector Form of Integral Conservation Laws

By using the vector notation defined above, the integral conservation laws defined in eqns. (9.7), (9.9), (9.11), (9.13), and (9.15) can be written in a single equation as

$$\begin{aligned} \mathbf{U}^{n+1}V^{n+1} - \mathbf{U}^nV^n = & - \int_{t^n}^{t^{n+1}} \left({}^{-i}(\text{con } \mathbf{F}) + {}^{+i}(\text{con } \mathbf{F}) + {}^{-j}(\text{con } \mathbf{F}) + {}^{+j}(\text{con } \mathbf{F}) + {}^{-k}(\text{con } \mathbf{F}) + {}^{+k}(\text{con } \mathbf{F}) \right) dt \\ & - \int_{t^n}^{t^{n+1}} \left({}^{-i}(\text{vis } \mathbf{F}) + {}^{+i}(\text{vis } \mathbf{F}) + {}^{-j}(\text{vis } \mathbf{F}) + {}^{+j}(\text{vis } \mathbf{F}) + {}^{-k}(\text{vis } \mathbf{F}) + {}^{+k}(\text{vis } \mathbf{F}) \right) dt \\ & + \int_{t^n}^{t^{n+1}} \mathbf{W} dt \end{aligned} \quad (9.25)$$

10. Chemical Reactions

At the regime of hypersonic flow, the atmosphere cannot be considered an ideal gas. A strong bow shock can dissociate molecules and breakdown of the thermal protection materials can further enrich the chemical “soup”. The chemical reactions between these various species must be modeled with a representative, though not necessarily exhaustive, system of rate equations. A standard discussion of gas flows can be found in Vicenti & Kreuger (1975). See Keenan (1994) for an example of one useful approach incorporating ablation. Havstad (2002) provides a comparison of multiple approaches employed in the planetary probe community. The topic of chemistry modeling will be addressed after the basic flow simulation code is operational.

11. Turbulence Models

Turbulence modeling is a complex subject that remains an area of active research. Different problem classes often yield to different approaches. The effect of turbulence can sometimes be

approximated at very little cost by using phenomenological models such as the algebraic turbulence model of Baldwin and Lomax (1978). A more sophisticated turbulence model may be required than that provided by the Baldwin-Lomax model. Roy and Blottner (2001) found that the turbulence model of Spalart and Allmaras (1992) provided reliable and accurate results for hypersonic flows. In addition to the turbulence model itself, an important issue for the current problem class is the location of the transition from laminar to turbulent flow in the boundary layer. The enhanced mixing in the turbulent portion of the boundary layer has the effect of increasing transport. The topic of turbulence modeling will be addressed during successive refinement of the flow simulation code.

12. Energy Exchange Mechanisms

Energy can be exchanged between the vibrational energies of the various species as well as with the translational thermal energy of the system. These effects are viewed as source terms in the balance laws considered in Sections 9.3 and 9.4. Incorporation of electron temperature as another nonequilibrium consideration would entail another balance law and further exchange mechanisms. Vincenti & Kreuger (1975) provide a standard discussion. See Candler (1988) and Keenan (1994) and follow on work for more contemporary applications.

13. Non-Inertial Reference Frame

A re-entry vehicle can experience large accelerations. In addition to the rapid deceleration caused by the aerodynamic drag on the vehicle, lateral accelerations may also occur. Furthermore, the vehicle may be spinning, and the spin may not be steady. The body-fixed computational coordinate system accelerates with the body. The fact that the coordinate system is accelerating means that it is *non-inertial*, or *non-Newtonian*. In a non-inertial reference frame Newton's laws do not appear to be valid. In particular, momentum is not conserved, and the usual conservation-law form of the fluid dynamic governing equations must be corrected in order to obtain accurate results.

A brief discussion of the effects of a non-inertial reference frame is provided in Batchelor (1967). It is shown that the usual conservation-law form of the fluid dynamic governing equations can be used for non-inertial reference frames if a fictitious body force is added to the momentum equations. This body force is therefore included in the source terms for the momentum equations given by eqn. (9.15), with

$$\vec{a} = {}^{org}\vec{a} + {}^{\alpha}\vec{a} + {}^{cor}\vec{a} + {}^{cen}\vec{a} \quad (13.1)$$

The first term in this equation is the linear acceleration of the origin of the non-inertial reference frame, the second term arises from the angular acceleration of the non-inertial reference frame, the third term is the coriolis acceleration, and the last term is the well-known centripetal acceleration. These terms depend on the motion of the non-inertial reference frame, and the motion of the fluid as follows:

$${}^{\alpha}\vec{a} = \vec{\alpha} \times \vec{r} \quad (13.2)$$

$${}^{cor}\vec{a} = 2\vec{\Omega} \times \vec{v} \quad (13.3)$$

$${}^{cen}\vec{a} = \vec{\Omega} \times (\vec{\Omega} \times \vec{r}) \quad (13.4)$$

where $\vec{\Omega}$ is the angular velocity of the noninertial reference frame, $\vec{\alpha}$ is the angular acceleration of the non-inertial reference frame, \vec{r} is the position vector from the origin of the noninertial reference frame to the fluid particle of interest, and \vec{v} , as usual, is the velocity of the fluid particle relative to the non-inertial reference frame. Equation (13.1) is a vector equation, and its individual components are required for use in eqn. (9.15). By using eqns. (13.2) (13.4) these components can be computed as

$$a_1 = {}^{org}a_1 + (\alpha_2 r_3 - \alpha_3 r_2) + 2(\Omega_2 v_3 - \Omega_3 v_2) + (\Omega_2(\Omega_1 r_2 - \Omega_2 r_1) - \Omega_3(\Omega_3 r_1 - \Omega_1 r_3)) \quad (13.5)$$

$$a_2 = {}^{org}a_2 + (\alpha_3 r_1 - \alpha_1 r_3) + 2(\Omega_3 v_1 - \Omega_1 v_3) + (\Omega_3(\Omega_2 r_3 - \Omega_3 r_2) - \Omega_1(\Omega_1 r_2 - \Omega_2 r_1)) \quad (13.6)$$

$$a_3 = {}^{org}a_3 + (\alpha_1 r_2 - \alpha_2 r_1) + 2(\Omega_1 v_2 - \Omega_2 v_1) + (\Omega_1(\Omega_3 r_1 - \Omega_1 r_3) - \Omega_2(\Omega_2 r_3 - \Omega_3 r_2)) \quad (13.7)$$

14. Nondimensionalization

It is good practice to use reference quantities to rewrite the governing equations in a nondimensional form. This procedure helps to reduce errors from finite precision arithmetic on digital computers. A reference length, density, temperature, and velocity are needed to define nondimensional variables. These are designated as ${}^{ref}L$, ${}^{ref}\rho$, ${}^{ref}T$, and ${}^{ref}v$. Then nondimensional variables can be defined as follows:

$$\hat{t} = \frac{t}{{}^{ref}L / {}^{ref}v} \quad (14.1)$$

$$\hat{x} = \frac{x}{{}^{ref}L} \quad (14.2)$$

$$\hat{\rho}^s = \frac{\rho^s}{{}^{ref}\rho} \quad (14.3)$$

$$\hat{v}_d = \frac{v_d}{{}^{ref}v} \quad (14.4)$$

$$\hat{p} = \frac{p}{{}^{ref}\rho {}^{ref}v^2} \quad (14.5)$$

The following nondimensional form applies to all energies:

$$\hat{E} = \frac{E}{\rho_{ref} v_{ref}^2} \quad (14.6)$$

The nondimensional form for the turbulence variables depends upon the nature of the turbulence model. For the Spalart-Allmaras model the turbulence variable is a kinematic viscosity, $\tilde{\nu}$. The appropriate nondimensional form is

$$\hat{\tilde{\nu}} = \frac{\tilde{\nu}}{v_{ref} L} \quad (14.7)$$

The nondimensional form of the source term in the Spalart-Allmaras turbulence model is

$${}^t\hat{W} = \frac{{}^tW}{\rho_{ref} v_{ref}^2} \quad (14.8)$$

Additional nondimensional forms are given below.

$$\hat{\tau}_{i,j} = \frac{\tau_{i,j}}{\rho_{ref} v_{ref}^2} \quad (14.9)$$

$$\hat{q} = \frac{q}{\rho_{ref} v_{ref}^3} \quad (14.10)$$

$$\hat{h} = \frac{h}{v_{ref}^2} \quad (14.11)$$

$$\hat{w}^s = \frac{w^s}{\rho_{ref} v_{ref} / L} \quad (14.12)$$

$$\hat{a}_d = \frac{a_d}{v_{ref}^2 / L} \quad (14.13)$$

$$\hat{e} = \frac{e}{v_{ref}^2} \quad (14.14)$$

$$\hat{T} = \frac{T}{T_{ref}} \quad (14.15)$$

$$\hat{c}_v = \frac{c_v}{v_{ref}^2 / T_{ref}} \quad (14.16)$$

$$\hat{R} = \frac{R}{v_{ref}^2 / T_{ref}} \quad (14.17)$$

$$\hat{\mu} = \frac{\mu}{\rho_{ref} v_{ref} L} \quad (14.18)$$

$$\hat{\kappa} = \frac{\kappa}{\rho_{ref} v_{ref}^2 L / T} \quad (14.19)$$

$$\hat{D} = \frac{D}{v_{ref} L} \quad (14.20)$$

The equations for the nondimensional form of the variables given above can be inverted to yield expressions for the dimensional variables in terms of the nondimensional variables and the reference quantities. These expressions can then be substituted into the governing equations to derive governing equations written with nondimensional variables. Groups of reference quantities appear in each term of the new governing equations. By dividing each term by this group of reference quantities the original form of the governing equations is recovered. Thus, the nondimensional form of the governing equations is identical to the dimensional form, with all dimensional quantities replaced with nondimensional quantities. The equations are not repeated here in the interest of brevity.

Since the new, nondimensional form of the governing equations is identical to the dimensional form, no further reference will be made to the dimensional form of the variables. For the remainder of this document, all variables will be regarded as nondimensional, all equations will be regarded as nondimensional, and the notational convention of using an arc over a variable to denote that it is nondimensional will be dropped.

The equations of state can be converted into a nondimensional form using the same procedure as was used for the governing equations. Generally, each equation of state converts into an identical equation with nondimensional quantities substituted for dimensional quantities. An exception to this occurs when curve fits of experimental data are used, as in eqn. (6.7). These equations must be used in their dimensional form, with the result divided by the appropriate reference quantities for subsequent use in other equations.

15. Spatial Reconstruction

We wish to introduce a computational flux that is a function of the conserved quantities \mathbf{U} . Recall that for the finite volume formulation the value of \mathbf{U} for a given cell is its average value in that cell. However, the computational flux vector is needed at the cell faces. Higher-order spatial accuracy is essential for good results, and in order to achieve higher-order spatial accuracy the value of \mathbf{U} at the cell faces must be “reconstructed” from the cell-average values, rather than merely setting it to a cell-average value. Much research has been devoted to methods for accomplishing this. For hypersonic flow, where extremely strong shocks are present, it is essential that the reconstruction method be robust in the presence of these strong shocks, and that the reconstruction method not induce any over- or under-shoots in the conserved quantities near the shocks.

After considerable experimentation with various methods on a 1-D Mach 20 normal shock model problem, the method described by Keenan (1994) was selected. The basic reconstruction has second-order spatial accuracy, but the reconstruction drops to first-order spatial accuracy in regions of strong pressure gradients. The strong pressure gradients are caused by shocks, and the lower order of accuracy near the shock provides robust shock capturing with no over- or under-shoots.

The reconstruction assumes a linear variation in the conserved quantities, with the slope set to zero in regions of strong pressure gradients

$${}^{-i}\mathbf{U} = \mathbf{U} + \frac{\psi}{2}(\mathbf{U} - \mathbf{U}_{i+1}) \quad (15.1)$$

$${}^{+i}\mathbf{U} = \mathbf{U} + \frac{\psi}{2}(\mathbf{U} - \mathbf{U}_{i-1}) \quad (15.2)$$

with similar expressions written in the obvious manner for ${}^{-j}\mathbf{U}$, ${}^{+j}\mathbf{U}$, ${}^{-k}\mathbf{U}$, and ${}^{+k}\mathbf{U}$.

The parameter ψ varies from 0 to 1, and is set based on the magnitude of the local pressure gradients. When ψ is near 1 (in most of the flow) the reconstruction has second-order accuracy, and when ψ drops to 0 near shocks, the method reduces to first-order accuracy. The method used to calculate ψ was modified from that given by Keenan in order to provide a more compact and symmetric stencil.

$$\begin{aligned} \psi = & \left(1 + k \max \left(\left(\frac{{}^{-i}\partial \bar{p}}{\partial \xi_1} \right)^2, \left(\frac{{}^{+i}\partial \bar{p}}{\partial \xi_1} \right)^2 \right) \right)^{-2} \\ & \times \left(1 + k \max \left(\left(\frac{{}^{-j}\partial \bar{p}}{\partial \xi_2} \right)^2, \left(\frac{{}^{+j}\partial \bar{p}}{\partial \xi_2} \right)^2 \right) \right)^{-2} \\ & \times \left(1 + k \max \left(\left(\frac{{}^{-k}\partial \bar{p}}{\partial \xi_3} \right)^2, \left(\frac{{}^{+k}\partial \bar{p}}{\partial \xi_3} \right)^2 \right) \right)^{-2} \end{aligned} \quad (15.3)$$

The normalized pressure gradients are

$$\left(\frac{{}^{-i}\partial \bar{p}}{\partial \xi_1} \right)^2 = \left(\frac{p - p_{i-1}}{\min(p, p_{i-1})} \right)^2 \quad (15.4)$$

$$\left(\frac{{}^{+i}\partial \bar{p}}{\partial \xi_1} \right)^2 = \left(\frac{p_{i+1} - p}{\min(p_{i+1}, p)} \right)^2 \quad (15.5)$$

$$\left(\frac{\partial p}{\partial \xi_2}\right)^2 = \left(\frac{p - p_{j-1}}{\min(p, p_{j-1})}\right)^2 \quad (15.6)$$

The other required normalized pressure gradients can be computed in a similar manner, taking care to always use appropriate data for the cell face of interest, and maintaining symmetry.

Spatial reconstruction is not used at the boundaries of the flow, and the method therefore reverts to first-order accuracy at the boundaries.

16. Convective Flux

A one-dimensional model problem was used to investigate various methods for calculating the convective fluxes. The model problem was a Mach 20 normal shock with an ideal gas. Many different schemes were evaluated with this model problem, which was intended to be representative of the stagnation streamline for a hypersonic bow shock. The best results were obtained with the flux difference vector splitting scheme of Roe (1986). The flux split scheme of Steger and Warming (1981) is also included to provide a lower cost (but less accurate) convective flux.

16.1 Flux Splitting

All flux-splitting methods depend on the existence of a Jacobian matrix that relates the convective flux to the conserved quantities.

$${}^{con}\mathbf{F} = {}^{con}\mathbf{A}\mathbf{U} \quad (16.1)$$

where

$${}^{con}\mathbf{A} = \frac{\partial {}^{con}\mathbf{F}}{\partial \mathbf{U}} \quad (16.2)$$

Note that the system of governing equations is said to be homogeneous if the above two equations are satisfied – not all real gas systems are homogeneous. However, the system considered here is homogeneous. It is simpler to compute the partial derivatives of the convective flux with respect to a set of primitive variables, instead of using eqn. (16.2) directly. Using the chain rule of matrix differentiation,

$${}^{con}\mathbf{A} = \frac{\partial {}^{con}\mathbf{F}}{\partial \mathbf{V}} \frac{\partial \mathbf{V}}{\partial \mathbf{U}} \quad (16.3)$$

where \mathbf{V} is the vector of primitive variables, to be defined shortly. By also defining

$$\mathbf{S} = \frac{\partial \mathbf{V}}{\partial \mathbf{U}} \quad (16.4)$$

and premultiplying eqn. (16.3) by the identity matrix $\mathbf{S}^{-1}\mathbf{S}$, the expression for ${}^{con}\mathbf{A}$ takes the form of a similarity transformation

$${}^{con}\mathbf{A} = \mathbf{S}^{-1} \frac{\partial \mathbf{V}}{\partial \mathbf{U}} \frac{\partial {}^{con}\mathbf{F}}{\partial \mathbf{V}} \mathbf{S} \quad (16.5)$$

16.2 Primitive Variables and Transformation Matrices

The choice of primitive variables is not unique, and the following selection was made to provide the simplest possible form for the subsequent eigenanalysis. The primitive variables are

$$\mathbf{V} = \left\{ \begin{array}{c} \rho^1 \\ \vdots \\ \rho^{NS} \\ \dots \\ {}^t u^1 \\ \vdots \\ {}^t u^{NT} \\ \dots \\ {}^v e^1 \\ \vdots \\ {}^v e^{NV} \\ \dots \\ p \\ \dots \\ v_1 \\ v_2 \\ v_3 \end{array} \right\} \quad (16.6)$$

In order to compute the matrix \mathbf{S} the primitive variables must be expressed in terms of the conserved quantities.

$$\mathbf{V}(\mathbf{U}) = \left\{ \begin{array}{c} \rho^1 \\ \vdots \\ \rho^{NS} \\ \hline {}^t u^1 \\ \vdots \\ {}^t u^{NT} \\ \hline {}^v E^1 / \rho^{vs(1)} \\ \vdots \\ {}^v E^{NV} / \rho^{vs(NV)} \\ \hline p(\mathbf{U}) \\ \hline m_1 \left(\sum_{s=1}^{NS} \rho^s \right)^{-1} \\ \hline m_2 \left(\sum_{s=1}^{NS} \rho^s \right)^{-1} \\ \hline m_3 \left(\sum_{s=1}^{NS} \rho^s \right)^{-1} \end{array} \right\} \quad (16.7)$$

Recall that the temperature (and, therefore, the pressure), cannot, in general, be explicitly expressed in terms of the conserved quantities (see Section 5). Thus, $p(\mathbf{U})$ in the above equation is implicitly defined by eqns. (5.12) and (5.13).

In order to compute the matrix \mathbf{S}^{-1} the conserved quantities must be expressed in terms of the primitive variables.

$$\mathbf{U}(\mathbf{V}) = \left\{ \begin{array}{c} \rho^1 \\ \vdots \\ \rho^{NS} \\ \hline {}^t u^1 \\ \vdots \\ {}^t u^{NT} \\ \hline {}^v e^1 \rho^{vs(1)} \\ \vdots \\ {}^v e^{NV} \rho^{vs(NV)} \\ \hline \sum_{s=1}^{NS} \rho^s \int_0^p \sum \rho^s R^s c_v^s(\theta) d\theta + \sum_{s=1}^{NS} \rho^s f h^s + \sum_{r=1}^{NV} {}^v e^r \rho^{vs(r)} + \frac{1}{2} \sum_{s=1}^{NS} \rho^s \sum_{d=1}^3 v_d^2 \\ \hline v_1 \sum_{s=1}^{NS} \rho^s \\ v_2 \sum_{s=1}^{NS} \rho^s \\ v_3 \sum_{s=1}^{NS} \rho^s \end{array} \right\} \quad (16.8)$$

Note that the temperature can be explicitly expressed in terms of the primitive variables, so no implicit terms appear in eqn. (16.8).

The matrix \mathbf{S} can now be defined by computing the partial derivatives defined by eqn. (16.4). Only the non-zero elements of \mathbf{S} are shown.

$$\mathbf{S} = \frac{\partial \mathbf{V}}{\partial \mathbf{U}} = \begin{bmatrix} 1 & & & & & & & & & & & & \\ & \ddots & & & & & & & & & & & \\ & & 1 & & & & & & & & & & \\ & & & 1 & & & & & & & & & \\ & & & & \ddots & & & & & & & & \\ & & & & & 1 & & & & & & & \\ & \frac{-^v e^l}{\rho^{vs(1)}} & & & & \frac{1}{\rho^{vs(1)}} & & & & & & & \\ & & \frac{-^v e^r}{\rho^{vs(r)}} & & & \frac{1}{\rho^{vs(r)}} & & & & & & & \\ & \frac{-^v e^{NV}}{\rho^{vs(NV)}} & & & & \frac{1}{\rho^{vs(NV)}} & & & & & & & \\ \frac{\partial p}{\partial \rho^1} & \dots & \frac{\partial p}{\partial \rho^{NS}} & & & -\beta & \dots & -\beta & \beta & -\beta v_1 & -\beta v_2 & -\beta v_3 \\ \frac{-v_1}{\rho} & \dots & \frac{-v_1}{\rho} & & & & & & \frac{1}{\rho} & & & & \\ \frac{-v_2}{\rho} & \dots & \frac{-v_2}{\rho} & & & & & & & \frac{1}{\rho} & & & \\ \frac{-v_3}{\rho} & \dots & \frac{-v_3}{\rho} & & & & & & & & \frac{1}{\rho} & & \end{bmatrix} \quad (16.9)$$

The partial derivatives of the pressure with respect to ρ^s are obtained by differentiating eqn. (5.13).

$$\frac{\partial p}{\partial \rho^s} = R^s T + \rho \bar{R} \frac{\partial T}{\partial \rho^s} \quad (16.10)$$

Implicit differentiation of the equation for the total energy expressed in terms of the conserved quantities provides the partial derivative of T with respect to ρ^s required for the above equation

$$E(\mathbf{U}) = \frac{\vec{m}^2}{2} \left(\sum_{s=1}^{NS} \rho^s \right)^{-1} + \sum_{r=1}^{NV} {}^v E^r + \sum_{s=1}^{NS} \rho^s \left({}^f h^s + \int_0^T c_v^s(\theta) d\theta \right) \quad (16.11)$$

$$\frac{\partial E(\mathbf{U})}{\partial \rho^s} \equiv 0 = {}^{eq} e^s + \rho \bar{c}_v \frac{\partial T}{\partial \rho^s} - \frac{\vec{v}^2}{2} \quad (16.12)$$

$$\frac{\partial T}{\partial \rho^s} = \frac{\frac{\vec{v}^2}{2} - {}^{eq} e^s}{\rho \bar{c}_v} \quad (16.13)$$

so that the final result is

$$\frac{\partial p}{\partial \rho^s} = R^s T + \beta \left(\frac{\vec{v}^2}{2} - {}^{eq}e^s \right) \quad (16.14)$$

with

$$\beta = \bar{\gamma} - 1 \quad (16.15)$$

The location of the $\frac{{}^v e^r}{\rho^{vs(r)}}$ terms in the \mathbf{S} matrix cannot be specified *a priori*, as the relationship between the nonequilibrium energies and their corresponding densities depends on the particular set of species present in a problem, and is therefore input-dependent. The irregular arrangement of these terms in eqn. (16.9) is intended to be a reminder of that fact. The column that contains $\frac{{}^v e^r}{\rho^{vs(r)}}$ can be found from the vibrational species index list as $vs(r)$.

The \mathbf{S}^{-1} matrix is defined by computing the partial derivatives of \mathbf{U} with respect to \mathbf{V} .

$$\mathbf{S}^{-1} = \frac{\partial \mathbf{U}}{\partial \mathbf{V}} = \begin{bmatrix} 1 & & & & & & & & & & \\ & \ddots & & & & & & & & & \\ & & 1 & & & & & & & & \\ & & & 1 & & & & & & & \\ & & & & \ddots & & & & & & \\ & & & & & 1 & & & & & \\ & {}^v e^1 & & & & \rho^{vs(1)} & & & & & \\ & & {}^v e^r & & & \rho^{vs(r)} & & & & & \\ & {}^v e^{NV} & & & & & \rho^{vs(NV)} & & & & \\ \frac{\partial E}{\partial \rho^1} & \cdots & \frac{\partial E}{\partial \rho^{NS}} & & & \rho^{vs(1)} & \cdots & \rho^{vs(NV)} & \frac{1}{\beta} & m_1 & m_2 & m_3 \\ v_1 & \cdots & v_1 & & & & & & \rho & & & \\ v_2 & \cdots & v_2 & & & & & & & \rho & & \\ v_3 & \cdots & v_3 & & & & & & & & \rho & \end{bmatrix} \quad (16.16)$$

with

$$\frac{\partial E(\mathbf{V})}{\partial \rho^s} = {}^{eq}e^s + {}^v e^{sv(s)} + \frac{\vec{v}^2}{2} - \frac{R^s T}{\beta} \quad (16.17)$$

Note that the vibrational energy in the above equation is the vibrational energy that corresponds to the density ρ^s . Some species may not have a corresponding vibrational energy (e.g.

monatomic species). The index list $sv(s)$, which is the inverse of the index list vs , provides the appropriate nonequilibrium energy number for species s .

The next matrix that is required is the partial derivative of the convective flux with respect to the primitive variables shown in eqn. (16.3). First, rewrite the convective flux vector, eqn. (9.16), in terms of the primitive variables, eqn. (16.6). Recall that

$$m_d(\mathbf{V}) = v_d \sum_{s=1}^{NS} \rho^s \quad (16.18)$$

$${}^v E^r(\mathbf{V}) = {}^v e^r \rho^{vs(r)} \quad (16.19)$$

$$E(\mathbf{V}) = \sum_{s=1}^{NS} \rho^s \int_0^{p/\sum \rho^s R^s} c_v^s(\theta) d\theta + \sum_{s=1}^{NS} \rho^s f h^s + \sum_{r=1}^{NV} {}^v e^r \rho^{vs(r)} + \frac{1}{2} \sum_{s=1}^{NS} \rho^s \sum_{d=1}^3 v_d^2 \quad (16.20)$$

substitution of these expressions into eqn. (9.16), and differentiation with respect to the primitive variables, gives

The matrix product $\mathbf{S} \frac{\partial^{con} \mathbf{F}}{\partial \mathbf{V}}$ needed for eqn. (16.5) can now be computed

$$\mathbf{S} \frac{\partial^{con} \mathbf{F}}{\partial \mathbf{V}} = \mathbf{S} \begin{bmatrix} \begin{matrix} e_v & & & & & \\ & \ddots & & & & \\ & & e_v & & & \\ & & & \ddots & & \\ & & & & e_v & \\ & & & & & \ddots \\ & & & & & & e_v \end{matrix} & \begin{matrix} \rho^l n_1 & \rho^l n_2 & \rho^l n_3 \\ \vdots & \vdots & \vdots \\ \rho^{NS} n_1 & \rho^{NS} n_2 & \rho^{NS} n_3 \\ {}^t u^l n_1 & {}^t u^l n_2 & {}^t u^l n_3 \\ \vdots & \vdots & \vdots \\ {}^t u^{NT} n_1 & {}^t u^{NT} n_2 & {}^t u^{NT} n_3 \end{matrix} \\ \begin{matrix} & & & e_v & & \\ & & & & \ddots & \\ & & & & & e_v \end{matrix} & \begin{matrix} \rho c^2 n_1 & \rho c^2 n_2 & \rho c^2 n_3 \\ n_1 / \rho & e_v & \\ n_2 / \rho & & e_v \\ n_3 / \rho & & & e_v \end{matrix} \end{bmatrix} \quad (16.22)$$

16.3 Convective Flux Eigensystem

The eigenvalues and eigenvectors of the matrix given by eqn. (16.22) are needed to allow for upwind differencing of the convective flux. With the matrix of eigenvectors defined as \mathbf{E} and the diagonal matrix of eigenvalues defined as $\boldsymbol{\lambda}$, we can write the resulting eigensystem as

$$\mathbf{S} \frac{\partial^{con} \mathbf{F}}{\partial \mathbf{V}} \mathbf{E} = \mathbf{E} \boldsymbol{\lambda} \quad (16.23)$$

By multiplying each side of this equation by the inverse of \mathbf{E} , we obtain

$$\mathbf{S} \frac{\partial^{con} \mathbf{F}}{\partial \mathbf{V}} = \mathbf{E} \boldsymbol{\lambda} \mathbf{E}^{-1} \quad (16.24)$$

The eigensystem matrices are given by

$$\lambda = S \begin{bmatrix} {}^e v & & & & & \\ & \ddots & & & & \\ & & {}^e v & & & \\ & & & \ddots & & \\ & & & & {}^e v & \\ & & & & & \ddots \\ & & & & & & {}^e v + c \\ & & & & & & & {}^e v - c \\ & & & & & & & & {}^e v \\ & & & & & & & & & {}^e v \end{bmatrix} \quad (16.25)$$

$$\mathbf{E} = \begin{bmatrix} 1 & & & & \rho^1/c & -\rho^1/c & & \\ & \ddots & & & \vdots & \vdots & & \\ & & 1 & & \rho^{NS}/c & -\rho^{NS}/c & & \\ & & & 1 & {}^t u^1/c & -{}^t u^1/c & & \\ & & & & \vdots & \vdots & & \\ & & & & {}^t u^{NT}/c & -{}^t u^{NT}/c & & \\ & & & & & & 1 & \\ & & & & & & & \ddots \\ & & & & & & & & 1 \\ & & & & & & & & & \rho c & -\rho c \\ & & & & & & & & & n_1 & n_1 & -n_2 & -n_3 \\ & & & & & & & & & n_2 & n_2 & n_1 & 0 \\ & & & & & & & & & n_3 & n_3 & 0 & n_1 \end{bmatrix} \quad (16.26)$$

$$\mathbf{E}^{-1} = \begin{bmatrix} 1 & & & & & & & -\rho^1/\rho c^2 \\ & \ddots & & & & & & \vdots \\ & & 1 & & & & & -\rho^{NS}/\rho c^2 \\ & & & \ddots & & & & -{}^t u^1/\rho c^2 \\ & & & & 1 & & & \vdots \\ & & & & & \ddots & & -{}^t u^{NT}/\rho c^2 \\ & & & & & & 1 & \\ & & & & & & & \ddots \\ & & & & & & & 1 \\ & & & & & & & & \frac{1}{2\rho c} & \frac{n_1}{2} & \frac{n_2}{2} & \frac{n_3}{2} \\ & & & & & & & & -\frac{1}{2\rho c} & \frac{n_1}{2} & \frac{n_2}{2} & \frac{n_3}{2} \\ & & & & & & & & & -n_2 & \frac{n_1^2 + n_3^2}{n_1} & -\frac{n_2 n_3}{n_1} \\ & & & & & & & & & & \frac{n_1^2 + n_2^2}{n_1} & \frac{n_2^2 + n_3^2}{n_1} \\ & & & & & & & & & & -n_3 & -\frac{n_2 n_3}{n_1} & \frac{n_1^2 + n_2^2}{n_1} \end{bmatrix} \quad (16.27)$$

Note that the four terms in the lower right corner of \mathbf{E}^{-1} have the term n_1 in their denominator. In general, there can be no assurance that this term will not be zero, so there is a potential divide-by-zero problem with the above definition of \mathbf{E}^{-1} . This difficulty will be eliminated by a symbolic multiplication of the eigensystem matrices in Section 16.6. This multiplication will cancel the n_1 terms in the denominator of elements of \mathbf{E}^{-1} with n_1 terms in the numerator of elements of \mathbf{E} .

16.4 Steger-Warming Flux Splitting

The Steger-Warming flux splitting method uses data from the left side of the flux boundary for positive eigenvalues, and data from the right side of the flux boundary for negative eigenvalues. Let the reconstructed values of the conserved variables on the two sides of the flux boundary be denoted by \mathbf{U}_L and \mathbf{U}_R , with the computational index increasing in the direction from \mathbf{U}_L to \mathbf{U}_R . For example, for a computation of the convective flux on an i face, \mathbf{U}_L would be ${}^+i\mathbf{U}_i$, and \mathbf{U}_R would be ${}^-i\mathbf{U}_{i+1}$ (see Section 15). Then the Steger-Warming convective flux is

$${}^{S-W}(\text{}^{con}\mathbf{F}) = {}^+\mathbf{A}\mathbf{U}_L + {}^-\mathbf{A}\mathbf{U}_R \quad (16.28)$$

where

$${}^+\mathbf{A} = \mathbf{S}^{-1}\mathbf{E} + \lambda\mathbf{E}^{-1}\mathbf{S} \quad (16.29)$$

is computed using data from \mathbf{U}_L , and

$$-\mathbf{A} = \mathbf{S}^{-1} \mathbf{E}^{-1} \boldsymbol{\lambda} \mathbf{E}^{-1} \mathbf{S} \quad (16.30)$$

is computed using data from \mathbf{U}_R , and with

$$\pm \boldsymbol{\lambda} = \mathbf{S} \begin{bmatrix} \pm \lambda_1 & & & & \\ & \ddots & & & \\ & & \pm \lambda_1 & & \\ & & & \ddots & \\ & & & & \pm \lambda_1 \\ & & & & & \pm \lambda_2 \\ & & & & & & \pm \lambda_3 \\ & & & & & & & \pm \lambda_1 \\ & & & & & & & & \pm \lambda_1 \end{bmatrix} \quad (16.31)$$

$$\pm \lambda_1 = \frac{{}^e v \pm \sqrt{{}^e v^2 + \varepsilon^2}}{2} \quad (16.32)$$

$$\pm \lambda_2 = \frac{{}^e v + c \pm \sqrt{({}^e v + c)^2 + \varepsilon^2}}{2} \quad (16.33)$$

$$\pm \lambda_3 = \frac{{}^e v - c \pm \sqrt{({}^e v - c)^2 + \varepsilon^2}}{2} \quad (16.34)$$

Where ε is a small number, typically 0.001 or less, used to ensure that the eigenvalues have continuous derivatives.

16.5 Roe's Flux Difference Splitting

Roe's flux difference splitting method is used to calculate the convective flux at the surfaces of the finite volume cells. Roe's flux is defined by

$${}^{con}\hat{\mathbf{F}} = \frac{1}{2} \left({}^{con}\mathbf{F}(\mathbf{U}_L) + {}^{con}\mathbf{F}(\mathbf{U}_R) \right) - \frac{1}{2} |\hat{\mathbf{A}}| (\mathbf{U}_R - \mathbf{U}_L) \quad (16.35)$$

with

$$|\hat{\mathbf{A}}| = \hat{\mathbf{S}}^{-1} \hat{\mathbf{E}} |\hat{\boldsymbol{\lambda}}| \hat{\mathbf{E}}^{-1} \hat{\mathbf{S}} \quad (16.36)$$

The diagonal matrix of the absolute values of the eigenvalues is

$$|\hat{\boldsymbol{\lambda}}| = \mathbf{S} \begin{bmatrix} |\hat{\lambda}_1| & & & & \\ & \ddots & & & \\ & & |\hat{\lambda}_1| & & \\ & & & \ddots & \\ & & & & |\hat{\lambda}_1| \\ & & & & & |\hat{\lambda}_2| \\ & & & & & & |\hat{\lambda}_3| \\ & & & & & & & |\hat{\lambda}_1| \\ & & & & & & & & |\hat{\lambda}_1| \end{bmatrix} \quad (16.37)$$

$$|\hat{\lambda}_1| = \sqrt{{}^e \hat{v}^2 + \varepsilon^2} \quad (16.38)$$

$$|\hat{\lambda}_2| = \sqrt{\left({}^e \hat{v} + \hat{c} \right)^2 + \varepsilon^2} \quad (16.39)$$

$$|\hat{\lambda}_3| = \sqrt{\left({}^e \hat{v} - \hat{c} \right)^2 + \varepsilon^2} \quad (16.40)$$

Where ε in the above expressions, typically 0.001 or less, ensures that all derivatives are continuous.

The carat symbol over the matrices in eqn. (16.36) indicates that the matrices are computed using special Roe-averaged variables. The flux computed with Roe's method provides exact solutions for the Riemann problem when these Roe-averaged quantities are used. Following the work of Grossman and Cinnella (1990), we have

$$\hat{\rho} = \sqrt{\rho_L \rho_R} \quad (16.41)$$

$$\hat{\rho}^s = \hat{\rho} \frac{\frac{\rho_L^s}{\rho_L} \sqrt{\rho_L} + \frac{\rho_R^s}{\rho_R} \sqrt{\rho_R}}{\sqrt{\rho_L} + \sqrt{\rho_R}} \quad (16.42)$$

$${}^t\hat{u}^n = \frac{{}^t u_L^n \sqrt{\rho_L} + {}^t u_R^n \sqrt{\rho_R}}{\sqrt{\rho_L} + \sqrt{\rho_R}} \quad (16.43)$$

$${}^v\hat{e}^r = \frac{\frac{{}^v E_L^r}{\rho_L} \sqrt{\rho_L} + \frac{{}^v E_R^r}{\rho_R} \sqrt{\rho_R}}{\sqrt{\rho_L} + \sqrt{\rho_R}} \quad (16.44)$$

$$\hat{\vec{v}} = \frac{\vec{v}_L \sqrt{\rho_L} + \vec{v}_R \sqrt{\rho_R}}{\sqrt{\rho_L} + \sqrt{\rho_R}} \quad (16.45)$$

$${}^{tot}\hat{h} = \frac{{}^{tot} h_L \sqrt{\rho_L} + {}^{tot} h_R \sqrt{\rho_R}}{\sqrt{\rho_L} + \sqrt{\rho_R}} \quad (16.46)$$

$${}^{eq}\hat{e}^s = \frac{{}^{eq} e_L^s \sqrt{\rho_L} + {}^{eq} e_R^s \sqrt{\rho_R}}{\sqrt{\rho_L} + \sqrt{\rho_R}} \quad (16.47)$$

$$\hat{T} = \frac{T_L \sqrt{\rho_L} + T_R \sqrt{\rho_R}}{\sqrt{\rho_L} + \sqrt{\rho_R}} \quad (16.48)$$

$$\hat{\bar{R}} = \frac{\bar{R}_L \sqrt{\rho_L} + \bar{R}_R \sqrt{\rho_R}}{\sqrt{\rho_L} + \sqrt{\rho_R}} \quad (16.49)$$

An effective local specific heat can be defined by

$${}^*c_v^s = \frac{1}{T_R - T_L} \int_{T_L}^{T_R} c_v^s(\theta) d\theta \quad (16.50)$$

We can then define

$${}^*\hat{c}_v = \sum_{s=1}^{NS} \frac{\hat{\rho}^s {}^*c_v^s}{\hat{\rho}} \quad (16.51)$$

$$\hat{\gamma} = 1 + \frac{\hat{\bar{R}}}{{}^*\hat{c}_v} \quad (16.52)$$

$$\hat{c}^2 = (\hat{\gamma} - 1) \left({}^{tot}\hat{h} - \frac{\hat{v}^2}{2} + {}^*\hat{c}_v \hat{T} - \sum_{s=1}^{NS} \frac{{}^{eq}\hat{e}^s \hat{\rho}^s}{\hat{\rho}} - \sum_{r=1}^{NV} {}^v\hat{e}^r \right) \quad (16.53)$$

16.6 Symbolic Multiplication of Eigensystem Matrices

To eliminate the potential divide-by-zero in the definition of \mathbf{E}^{-1} as described in Section 16.3, the eigensystem matrices are symbolically multiplied as indicated in eqn. (16.24). The eigenvalues $\lambda_1, \lambda_2, \lambda_3$ are kept in evidence while this multiplication is carried out. This allows any flux-splitting scheme to use the symbolically-multiplied system, just by substituting in the appropriate eigenvalues.

17. Viscous Flux

This section will be expanded during subsequent development. Initially the simulation capability will be restricted to inviscid flows.

18. Flux Jacobians

The Jacobian of the flux is composed of a convective term and a viscous term. Addressing the convective terms first, it can be seen from eqn. (16.28) that the flux Jacobians for the Steger-Warming method are just the previously-defined $^+ \mathbf{A}$ and $^- \mathbf{A}$ matrices.

$$\frac{\partial^{S-W}({}^{con}\mathbf{F})}{\partial \mathbf{U}_L} = {}^+ \mathbf{A} \quad (18.1)$$

$$\frac{\partial^{S-W}({}^{con}\mathbf{F})}{\partial \mathbf{U}_R} = {}^- \mathbf{A} \quad (18.2)$$

For Roe's flux difference splitting method the Jacobians are computed by differentiating eqn. (16.35) with respect to \mathbf{U}_L and \mathbf{U}_R .

$$\frac{\partial {}^{con}\hat{\mathbf{F}}}{\partial \mathbf{U}_L} = \frac{1}{2} \left(\frac{\partial {}^{con}\mathbf{F}(\mathbf{U}_L)}{\partial \mathbf{U}_L} + |\hat{\mathbf{A}}| \right) = \frac{1}{2} \left({}^{con}\mathbf{A}(\mathbf{U}_L) + |\hat{\mathbf{A}}| \right) \equiv {}^+ \hat{\mathbf{A}} \quad (18.3)$$

$$\frac{\partial {}^{con}\hat{\mathbf{F}}}{\partial \mathbf{U}_R} = \frac{1}{2} \left(\frac{\partial {}^{con}\mathbf{F}(\mathbf{U}_R)}{\partial \mathbf{U}_R} - |\hat{\mathbf{A}}| \right) = \frac{1}{2} \left({}^{con}\mathbf{A}(\mathbf{U}_R) - |\hat{\mathbf{A}}| \right) \equiv {}^- \hat{\mathbf{A}} \quad (18.4)$$

The Jacobian of the convective flux, ${}^{con}\mathbf{A}$, is

Note that some methods that use Roe's flux-difference splitting have found the use of the simpler Steger-Warming Jacobians in the implicit time integration method provides adequate results at lower cost.

The eventual incorporation of viscous terms will augment the definitions of the $^+ \mathbf{A}$ and $^- \mathbf{A}$ matrices.

19. Source Terms

Deferred for subsequent development.

20. Source Jacobians

Deferred for subsequent development.

21. Time Integration

21.1 Second-Order Time Accuracy

Several approximations to the time integrals on the right hand side of eqn. (9.25) are possible. Using the source term in the conservation of mass equation as an example, we can define an explicit Euler time-integration scheme with

$$\int_{t^n}^{t^{n+1}} \dot{\rho}^s(t) V(t) dt = (\dot{\rho}^s V)^n \Delta t + O(\Delta t) \quad (21.1)$$

with

$$\Delta t = t^{n+1} - t^n \quad (21.2)$$

This scheme is only 1st-order accurate in time, and the size of the time step is limited by the CFL condition. An implicit Euler scheme is defined by evaluating the terms inside the time integrals at time t^{n+1} , and this change eliminates the CFL restriction. However, the implicit Euler method is still only 1st-order accurate in time. If the terms in the integrand are evaluated at the mid point of the time interval then 2nd-order time accuracy is achieved. This approach corresponds to Gaussian integration at the Gauss point of the time interval.

$$\int_{t^n}^{t^{n+1}} \dot{\rho}^s(t) V(t) dt = (\dot{\rho}^s V)^{n+1/2} \Delta t + O(\Delta t^2) \quad (21.3)$$

An equivalent formulation that also provides 2nd-order time accuracy is obtained by using the mean of the integrand's value at the beginning and the end of the time step. This approach corresponds to the trapezoidal rule of integration. The two formulations are identical if the integrands vary linearly with time

$$\int_{t^n}^{t^{n+1}} \dot{\rho}^s(t) V(t) dt = \frac{1}{2} \left((\dot{\rho}^s V)^n + (\dot{\rho}^s V)^{n+1} \right) \Delta t + O(\Delta t^2) \quad (21.4)$$

21.2 Implicit Formulation

Applying the trapezoidal rule integration method to the full set of conservation laws, eqn. (9.25), yields

$$\begin{aligned} \mathbf{U}^{n+1} V^{n+1} - \mathbf{U}^n V^n = & -\frac{\Delta t}{2} \left({}^{-i}\mathbf{F}^n + {}^{+i}\mathbf{F}^n + {}^{-j}\mathbf{F}^n + {}^{+j}\mathbf{F}^n + {}^{-k}\mathbf{F}^n + {}^{+k}\mathbf{F}^n \right) \\ & -\frac{\Delta t}{2} \left({}^{-i}\mathbf{F}^{n+1} + {}^{+i}\mathbf{F}^{n+1} + {}^{-j}\mathbf{F}^{n+1} + {}^{+j}\mathbf{F}^{n+1} + {}^{-k}\mathbf{F}^{n+1} + {}^{+k}\mathbf{F}^{n+1} \right) \\ & + \frac{\Delta t}{2} \mathbf{W}^n + \frac{\Delta t}{2} \mathbf{W}^{n+1} \end{aligned} \quad (21.5)$$

where the total flux \mathbf{F} is defined as the sum of the convective and viscous fluxes

$$\mathbf{F} = {}^{con}\mathbf{F} + {}^{vis}\mathbf{F} \quad (21.6)$$

Equation (21.5) can be simplified by defining the residual as

$$\mathbf{R} = \mathbf{W}^n - \left({}^{-i}\mathbf{F}^n + {}^{+i}\mathbf{F}^n + {}^{-j}\mathbf{F}^n + {}^{+j}\mathbf{F}^n + {}^{-k}\mathbf{F}^n + {}^{+k}\mathbf{F}^n \right) \quad (21.7)$$

so that

$$\mathbf{U}^{n+1} V^{n+1} - \mathbf{U}^n V^n = \frac{\Delta t}{2} \left(\mathbf{R} + \mathbf{W}^{n+1} - \left({}^{-i}\mathbf{F}^{n+1} + {}^{+i}\mathbf{F}^{n+1} + {}^{-j}\mathbf{F}^{n+1} + {}^{+j}\mathbf{F}^{n+1} + {}^{-k}\mathbf{F}^{n+1} + {}^{+k}\mathbf{F}^{n+1} \right) \right) \quad (21.8)$$

The volume terms in the above equation are not regarded as functions of the fluid variables, and are specified as a function of time. However, the flux and source terms are unknown at time step $n+1$, so they must be approximated with a linear expansion about their values at time n .

$$\mathbf{F}^{n+1} \approx \mathbf{F}^n + \left(\frac{\partial \mathbf{F}}{\partial \mathbf{U}} \right)^n (\mathbf{U}^{n+1} - \mathbf{U}^n) = \mathbf{F}^n + \mathbf{A} \delta \mathbf{U} \quad (21.9)$$

$$\mathbf{W}^{n+1} \approx \mathbf{W}^n + \left(\frac{\partial \mathbf{W}}{\partial \mathbf{U}} \right)^n (\mathbf{U}^{n+1} - \mathbf{U}^n) = \mathbf{W}^n + \mathbf{B} \delta \mathbf{U} \quad (21.10)$$

where the flux Jacobian, \mathbf{A} , and the source term Jacobian, \mathbf{B} , were previously defined in Sections 18 and 20, respectively, and

$$\delta \mathbf{U} = \mathbf{U}^{n+1} - \mathbf{U}^n \quad (21.11)$$

By substituting these expressions into eqn. (21.8) we obtain

$$\delta \mathbf{U} V^{n+1} - \mathbf{U}^n (V^n - V^{n+1}) = \Delta t \mathbf{R} + \frac{\Delta t}{2} \mathbf{B} \delta \mathbf{U} - \frac{\Delta t}{2} \left(\mathbf{A}^{-i} \delta \mathbf{U} + \mathbf{A}^{+i} \delta \mathbf{U} + \mathbf{A}^{-j} \delta \mathbf{U} + \mathbf{A}^{+j} \delta \mathbf{U} + \mathbf{A}^{-k} \delta \mathbf{U} + \mathbf{A}^{+k} \delta \mathbf{U} \right) \quad (21.12)$$

where

$$\mathbf{A}^{-i} \delta \mathbf{U} = \mathbf{A}_i^- \delta \mathbf{U}_{L,i} + \mathbf{A}_i^+ \delta \mathbf{U}_{R,i} \quad (21.13)$$

$$\mathbf{A}^{+i} \delta \mathbf{U} = \mathbf{A}_{i+1}^+ \delta \mathbf{U}_{L,i+1} + \mathbf{A}_{i+1}^- \delta \mathbf{U}_{R,i+1} \quad (21.14)$$

and similarly for the j and k faces. The i and $i+1$ subscripts in the above expressions refer to the indices of the flux boundaries. Recall that the flux boundary at the $-i$ face has the index i , and the flux boundary at the $+i$ face has the index $i+1$ (see Section 8.3). Since reconstruction is used to provide second-order spatial accuracy, $\delta \mathbf{U}_L$ and $\delta \mathbf{U}_R$ each contain data from 2 different cells

$$\delta \mathbf{U}_{L,i} = \delta \mathbf{U}_{i-1} + \frac{\psi_{i-1}}{2} (\delta \mathbf{U}_{i-1} - \delta \mathbf{U}_{i-2}) \quad (21.15)$$

$$\delta \mathbf{U}_{L,i+1} = \delta \mathbf{U}_i + \frac{\psi_i}{2} (\delta \mathbf{U}_i - \delta \mathbf{U}_{i-1}) \quad (21.16)$$

$$\delta \mathbf{U}_{R,i} = \delta \mathbf{U}_i + \frac{\psi_i}{2} (\delta \mathbf{U}_i - \delta \mathbf{U}_{i+1}) \quad (21.17)$$

$$\delta \mathbf{U}_{R,i+1} = \delta \mathbf{U}_{i+1} + \frac{\psi_{i+1}}{2} (\delta \mathbf{U}_{i+1} - \delta \mathbf{U}_{i+2}) \quad (21.18)$$

Note that the indices for the $\delta \mathbf{U}$ terms on the left hand side of the above equations refer to flux boundaries, whereas the indices for the $\delta \mathbf{U}$ terms on the right hand side refer to cells. The indices on the ψ terms refer to cells.

Most implicit methods neglect all terms on the right hand side of eqns. (21.15) – (21.18) except for the leading term. The resulting system of equations is more compact, with reduced bandwidth. The overall spatial accuracy of the method is unaffected by this approximation since the full reconstruction method is used in the calculation of the residual \mathbf{R} . However, one would expect that convergence to the correct solution would be more rapid if the effect of the reconstruction on the implicit terms were retained, and the full expressions will therefore be used here.

Substitution of eqns. (21.13) – (21.18), and their j and k counterparts, into eqn. (21.12), gives

$$\begin{aligned}
& {}^{i-2}\mathbf{D}\delta\mathbf{U}_{i-2} + {}^{i-1}\mathbf{D}\delta\mathbf{U}_{i-1} + {}^{i+1}\mathbf{D}\delta\mathbf{U}_{i+1} + {}^{i+2}\mathbf{D}\delta\mathbf{U}_{i+2} \\
& + {}^{j-2}\mathbf{D}\delta\mathbf{U}_{j-2} + {}^{j-1}\mathbf{D}\delta\mathbf{U}_{j-1} + {}^{j+1}\mathbf{D}\delta\mathbf{U}_{j+1} + {}^{j+2}\mathbf{D}\delta\mathbf{U}_{j+2} \\
& + {}^{k-2}\mathbf{D}\delta\mathbf{U}_{k-2} + {}^{k-1}\mathbf{D}\delta\mathbf{U}_{k-1} + {}^{k+1}\mathbf{D}\delta\mathbf{U}_{k+1} + {}^{k+2}\mathbf{D}\delta\mathbf{U}_{k+2} \\
& + \mathbf{D}\delta\mathbf{U} = \Delta t \mathbf{R} + \mathbf{U}^n (V^n - V^{n+1})
\end{aligned} \tag{21.19}$$

where

$$\mathbf{D} = V^{n+1} \mathbf{I} + \frac{\Delta t}{2} \left(\left(1 + \frac{\psi_i}{2} \right) ({}^+\mathbf{A}_{i+1} + {}^-\mathbf{A}_i + {}^+\mathbf{A}_{j+1} + {}^-\mathbf{A}_j + {}^+\mathbf{A}_{k+1} + {}^-\mathbf{A}_k) - \mathbf{B} \right) \tag{21.20}$$

$${}^{i-2}\mathbf{D} = -\frac{\Delta t}{2} \frac{\psi_{i-1}}{2} \mathbf{A}_i \tag{21.21}$$

$${}^{i-1}\mathbf{D} = -\frac{\Delta t}{2} \left(\left(1 + \frac{\psi_{i-1}}{2} \right) {}^+\mathbf{A}_i - \frac{\psi_i}{2} {}^+\mathbf{A}_{i+1} \right) \tag{21.22}$$

$${}^{i+1}\mathbf{D} = \frac{\Delta t}{2} \left(-\frac{\psi_i}{2} \mathbf{A}_i + \left(1 + \frac{\psi_{i+1}}{2} \right) {}^-\mathbf{A}_{i+1} \right) \tag{21.23}$$

$${}^{i+2}\mathbf{D} = -\frac{\Delta t}{2} \frac{\psi_{i+1}}{2} \mathbf{A}_{i+1} \tag{21.24}$$

and with the various \mathbf{D} terms defined similarly for the j and k directions.

By collecting the \mathbf{D} terms for every mesh cell into a single matrix, and collecting the right hand side terms in eqn. (21.19) for every cell into a right hand side vector, the resulting linear system can be solved for the change in the conserved quantities, $\delta\mathbf{U}$. Unfortunately, this solution procedure is impractical for two reasons. First, the bandwidth of the matrix will be large since off-diagonal terms occur in the i, j , and k directions. If the effect of the reconstruction is ignored this problem is not quite as severe, since the $i \pm 2$, $j \pm 2$, and $k \pm 2$ terms no longer appear in the matrix equation that must be solved. But it can still be impractical to solve this system directly. The second difficulty with the above formulation arises when a massively-parallel computer is used to solve the system. Such systems normally use distributed memory, and off-diagonal terms in the linear system cause the solutions on the various processors to be coupled. This greatly increases code complexity, and can significantly reduce parallel efficiency.

21.3 Data-Parallel Line Relaxation Method

The Data-Parallel Line Relaxation (DPLR) method developed by Wright, *et al.* (1998) eliminates the difficulties described above by recognizing that the need to adequately resolve the viscous boundary layer results in mesh cell sizes in the direction normal to the surface being much

smaller than the mesh cell sizes in the other directions. It is these extremely thin cells at the body surface that benefit most from the elimination of the CFL restriction of an explicit method. In the present development the DPLR method is extended to include the extra terms that arise from the spatial reconstruction.

Assume for the following development that the i direction is normal to the body surface. The method proceeds in an analogous manner for the j or k directions. By neglecting the j and k terms on the left hand side of eqn. (21.19) we obtain

$${}^{i-2}\mathbf{D}\delta\mathbf{U}_{i-2} + {}^{i-1}\mathbf{D}\delta\mathbf{U}_{i-1} + \mathbf{D}\delta\mathbf{U} + {}^{i+1}\mathbf{D}\delta\mathbf{U}_{i+1} + {}^{i+2}\mathbf{D}\delta\mathbf{U}_{i+2} = \Delta t \mathbf{R} + \mathbf{U}^n (V^n - V^{n+1}) \quad (21.25)$$

Denote the solution of this block-pentadiagonal system $\delta\mathbf{U}^0$. Then move the j and k terms on the left hand side of eqn. (21.19) to the right hand side, and take m_{\max} relaxation steps solving

$$\begin{aligned} {}^{i-2}\mathbf{D}\delta\mathbf{U}_{i-2}^m + {}^{i-1}\mathbf{D}\delta\mathbf{U}_{i-1}^m + \mathbf{D}\delta\mathbf{U}^m + {}^{i+1}\mathbf{D}\delta\mathbf{U}_{i+1}^m + {}^{i+2}\mathbf{D}\delta\mathbf{U}_{i+2}^m &= \Delta t \mathbf{R} \\ &+ \mathbf{U}^n (V^n - V^{n+1}) \\ &- {}^{j-2}\mathbf{D}\delta\mathbf{U}_{j-2}^{m-1} - {}^{j-1}\mathbf{D}\delta\mathbf{U}_{j-1}^{m-1} - {}^{j+1}\mathbf{D}\delta\mathbf{U}_{j+1}^{m-1} - {}^{j+2}\mathbf{D}\delta\mathbf{U}_{j+2}^{m-1} \\ &- {}^{k-2}\mathbf{D}\delta\mathbf{U}_{k-2}^{m-1} - {}^{k-1}\mathbf{D}\delta\mathbf{U}_{k-1}^{m-1} - {}^{k+1}\mathbf{D}\delta\mathbf{U}_{k+1}^{m-1} - {}^{k+2}\mathbf{D}\delta\mathbf{U}_{k+2}^{m-1} \end{aligned} \quad (21.26)$$

for $\delta\mathbf{U}^m$. Finally, update the conserved quantities with the results from the last relaxation step.

$$\mathbf{U}^{n+1} = \mathbf{U}^n + \delta\mathbf{U}^{m_{\max}} \quad (21.27)$$

The relaxation steps are very fast, since the previously factored linear system is used for each step, and only a simple back-substitution is required. Numerical studies described in Wright, *et al.* (1998) show that the DPLR method provides robust and rapid convergence, but with a somewhat higher usage of memory than some alternative methods.

22. Boundary Conditions

Boundary condition enforcement using the method of characteristic will be deferred to subsequent development.

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0.1	Aug. 21, 2002	Initial draft.
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0.3	Dec. 11, 2002	Revised finite-volume formulation.
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